

=====Structures for Co in a line=====

Ti O Ti O Ti O

1.000000000000000

14.2453041077000009 0.0000000000000000 0.0000000000000000

0.0000000000000000 5.1680002212999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 29.4789562224999990

Ti O H Co

21 57 18 3

Selective dynamics

Direct

0.0216197687200039 0.1096237504492837 0.3675231618423055 T T T

0.1847539701340245 0.6325978649533022 0.3963167743428571 T T T

0.5227720238545713 0.3986881667168366 0.3655715994556412 T T T

0.7662527485074795 0.3482319157011513 0.3661913095958659 T T T

0.9357827090182096 0.6355782074540109 0.3972586843320722 T T T

0.4401179092945225 0.8635185892449655 0.3990820399994366 T T T

0.2732524802462901 0.1559994783333669 0.3640569693744956 T T T

0.7342005810289152 0.1367530326270341 0.4848529224897646 F F F

0.3956158154875027 0.8683481241609385 0.5172283169192724 F F F

0.8953822014665107 0.6325289816178099 0.5172296942882255 F F F

0.2344372928950307 0.3634625181788707 0.4844606095791164 F F F

0.4815241771643173 0.3615968561732217 0.4834047030315531 F F F

0.1487325421792534 0.8563983739423122 0.5193773182996253 F F F

0.9814354254124780 0.1396032612863678 0.4834948480823442 F F F

0.4431524226628079 0.1433028417340188 0.6057217836950287 T T T

0.1070545655306835 0.8948070428401654 0.6382740522958537 T T T

0.9429493988654193 0.3687817529984496 0.6063470856448846 T T T

0.1857243801766117 0.3671984497422467 0.6052783566668160 T T T

0.3562851546590927 0.6581777570264477 0.6365369802559485 T T T

0.8545306826061789	0.8482835271939764	0.6380415546455876	T	T	T
0.6885487932725534	0.1387183196852257	0.6011157233300464	T	T	T
0.6661321210410593	0.1265917530200485	0.7281696688101024	T	T	T
0.9686905980040457	0.8195217685401884	0.3416710007405169	T	T	T
0.7470988618710822	0.1681948753329895	0.4205899540812044	T	T	T
0.2506963898833365	0.3129004931459590	0.4209990122216860	T	T	T
0.4729575374300235	0.6901078327110104	0.3417108937417400	T	T	T
0.8036709210185529	0.6869488574231538	0.3965900189258663	T	T	T
0.8997522180091999	0.3176570051156936	0.3647375309778372	T	T	T
0.4078500838842612	0.1804422783490328	0.3634536372317361	T	T	T
0.3092965471880907	0.8140717614366729	0.3961804349894820	T	T	T
0.0651618431845096	0.4634815445958202	0.3897589990059942	T	T	T
0.6471121294843247	0.5429608693501773	0.3726041642022689	T	T	T
0.1472997545753010	0.9660013296316307	0.3689858613954371	T	T	T
0.5720565547680230	0.0291166764248361	0.3940516305268593	T	T	T
0.7205891428266177	0.0312562129855282	0.3400888186704688	T	T	T
0.9842125437468927	0.9648267774114330	0.4235960018728188	T	T	T
0.4837893960044437	0.5318797715789789	0.4233188695004504	T	T	T
0.2299499064703042	0.4591353732246009	0.3391905050827329	T	T	T
0.6690919997630900	0.8170932275262288	0.4621108699766978	F	F	F
0.4563443067348629	0.1856957460417874	0.5415381954083784	F	F	F
0.9563715435325619	0.3157762323396867	0.5415514049333012	F	F	F
0.1684768759925106	0.6845410757490313	0.4614047933963619	F	F	F
0.5163401794135183	0.6840621747006708	0.5172222351935218	F	F	F
0.6122121268392959	0.3153938228045661	0.4863254931615089	F	F	F
0.1121104352761861	0.1862923125396918	0.4862169103188876	F	F	F
0.0164653504910319	0.8169379209085434	0.5170864510602016	F	F	F
0.7737086930159478	0.4642121896258828	0.5098542901532497	F	F	F
0.3547568199701061	0.5398845750144545	0.4913055491984935	F	F	F

0.8548352112812623	0.9612879754852131	0.4913474116743402	F	F	F
0.2736558171006749	0.0367285287095171	0.5095842622449496	F	F	F
0.4364578605973435	0.0348585244096000	0.4598389770138454	F	F	F
0.6931547229194095	0.9653791778681509	0.5438751113830449	F	F	F
0.1930960752500894	0.5368671613790212	0.5435284188581946	F	F	F
0.9363025789852344	0.4660265976351923	0.4598071447971463	F	F	F
0.3715851149702148	0.8229133973368971	0.5810479674123120	T	T	T
0.1559573655189703	0.1896480833200910	0.6617443132571010	T	T	T
0.6550619079826285	0.3506091015847795	0.6537265794363890	T	T	T
0.8752870768066288	0.6864475800021701	0.5814752625456077	T	T	T
0.2232179055970517	0.6865782036976644	0.6411148333713017	T	T	T
0.3193256237454277	0.3156482920045517	0.6094090236357069	T	T	T
0.8187423988782695	0.1877966526167031	0.6061276929666630	T	T	T
0.7176943564661039	0.8312200773059772	0.6387530621326003	T	T	T
0.4850185856903820	0.4755194644041293	0.6261293435001563	T	T	T
0.0615262355511959	0.5382641065084199	0.6100587992658417	T	T	T
0.5620481397697593	0.9622534555960929	0.6094526064537140	T	T	T
0.9784564028988532	0.0362474089757333	0.6342565640944012	T	T	T
0.1440889197777380	0.0349249948243757	0.5799356211006622	T	T	T
0.4088013182512558	0.9526502076714913	0.6641526998288076	T	T	T
0.9019863838856994	0.5468854566089885	0.6641156723272045	T	T	T
0.6437105316243037	0.4950034550474824	0.5757932980774880	T	T	T
0.0684666118928621	0.6815802344258409	0.6989032611603236	T	T	T
0.3683420865119935	0.4354659001189417	0.7013918238822394	T	T	T
0.8473802368078415	0.0694590546650026	0.7008713973572284	T	T	T
0.5611147485799145	0.7413248799695409	0.6929801413721877	T	T	T
0.2772645932123505	0.9234875625207897	0.3011546573557338	T	T	T
0.5622284274567351	0.1758756425582861	0.3057206056016342	T	T	T
0.7693320756690584	0.5738239109440320	0.3012765155403280	T	T	T

0.0325350601814875	0.3140102741714952	0.2996803355653139	T	T	T
0.0020755893576615	0.6257319483623451	0.6920680117170686	T	T	T
0.3717021376605588	0.2484964470537770	0.6926068954748879	T	T	T
0.8665412501331921	0.2495100944056221	0.6930120018249295	T	T	T
0.6049809998803946	0.8704685731160513	0.7070826525346756	T	T	T
0.1052693622577943	0.5202144162680403	0.6970202500000061	T	T	T
0.4311944887693758	0.4763236659817092	0.7126605548998264	T	T	T
0.7834592626751896	0.0832678094972225	0.7144599801091631	T	T	T
0.5019626873547670	0.8454482787543728	0.6843618105787769	T	T	T
0.2218419450110774	0.9677016374418199	0.2833698721390455	T	T	T
0.2670544755518007	0.7389161222097760	0.3112079149477058	T	T	T
0.5187961687292284	0.0271982341891405	0.3066405616603987	T	T	T
0.6252229909492599	0.0994791567545229	0.3163684186537437	T	T	T
0.7585050573158308	0.7559147734740439	0.3131833748631557	T	T	T
0.7127040769673326	0.5349594854340040	0.2839627894868713	T	T	T
0.0257497254397581	0.4962093269383656	0.3097452043426803	T	T	T
0.9726700016631037	0.2757075424472966	0.2850336997413246	T	T	T
0.6555432428920039	0.2462217451477669	0.7000955996321834	T	T	T
0.6474926305089040	0.2226798655934371	0.7550120671317211	T	T	T
0.6041463636148582	0.6370695829102657	0.6306693488107292	T	T	T
0.6487817750305567	0.6455289705310605	0.5195024736345744	F	F	F
0.6856132352173946	0.8710157122815668	0.3983476098242991	T	T	T

Ti O Ti O Ti O

1.0000000000000000

14.2453041077000009 0.0000000000000000 0.0000000000000000

0.0000000000000000 5.1680002212999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 29.4789562224999990

Ti O H Co

21 57 17 3

## Selective dynamics

### Direct

0.0211272469742708	0.1080687597439861	0.3672272625270711	T	T	T
0.1838278112071819	0.6318987598127783	0.3965077434098621	T	T	T
0.5219408244235731	0.4008163325077759	0.3652442361109206	T	T	T
0.7661832330125032	0.3482009722087122	0.3660044994984495	T	T	T
0.9356081676886115	0.6347186803085464	0.3976324729434892	T	T	T
0.4386443116502351	0.8634524047652470	0.3994305388135139	T	T	T
0.2726487543620675	0.1566462504661819	0.3638621412942209	T	T	T
0.7342005810289152	0.1367530326270341	0.4848529224897646	F	F	F
0.3956158154875027	0.8683481241609385	0.5172283169192724	F	F	F
0.8953822014665107	0.6325289816178099	0.5172296942882255	F	F	F
0.2344372928950307	0.3634625181788707	0.4844606095791164	F	F	F
0.4815241771643173	0.3615968561732217	0.4834047030315531	F	F	F
0.1487325421792534	0.8563983739423122	0.5193773182996253	F	F	F
0.9814354254124780	0.1396032612863678	0.4834948480823442	F	F	F
0.4404056804358871	0.1475077029100607	0.6058247021570666	T	T	T
0.1074976095857299	0.8965752303609941	0.6381576526416782	T	T	T
0.9431224292811945	0.3736552402671741	0.6064609137156851	T	T	T
0.1861204851297202	0.3694642352839763	0.6056310097103914	T	T	T
0.3575285090830072	0.6655806990405853	0.6376777391814712	T	T	T
0.8556367785859563	0.8518447070044394	0.6390462111325890	T	T	T
0.6887332251032411	0.1386012307853834	0.6019232245785764	T	T	T
0.6797636579642108	0.0805792356102659	0.7323267991911838	T	T	T
0.9684245522046837	0.8179795379682316	0.3416208379136479	T	T	T
0.7465965756077910	0.1684360282747525	0.4205112115379542	T	T	T
0.2502812248784672	0.3127100147833372	0.4208697796260396	T	T	T
0.4724346721080728	0.6917749196459498	0.3416066037915403	T	T	T

0.8032464861389947	0.6865557070056451	0.3966519793578698	T	T	T
0.8994102418743468	0.3171139177257878	0.3649057337730269	T	T	T
0.4077262202496574	0.1801496622850626	0.3637172864849474	T	T	T
0.3089635923961616	0.8132157803498473	0.3962757251615864	T	T	T
0.0648308685676235	0.4630613832866796	0.3897772135921910	T	T	T
0.6468092813398646	0.5429040759464561	0.3724131404693244	T	T	T
0.1471039671228920	0.9657108760385028	0.3689399775216146	T	T	T
0.5726638966839764	0.0268118462129108	0.3939929487638693	T	T	T
0.7205934033805269	0.0312038589370327	0.3399983037424009	T	T	T
0.9839602022156085	0.9643088190577758	0.4234535240100034	T	T	T
0.4836605854735965	0.5316189927844664	0.4231969630776155	T	T	T
0.2298953287389357	0.4592619453286159	0.3390645893404509	T	T	T
0.6690919997630900	0.8170932275262288	0.4621108699766978	F	F	F
0.4563443067348629	0.1856957460417874	0.5415381954083784	F	F	F
0.9563715435325619	0.3157762323396867	0.5415514049333012	F	F	F
0.1684768759925106	0.6845410757490313	0.4614047933963619	F	F	F
0.5163401794135183	0.6840621747006708	0.5172222351935218	F	F	F
0.6122121268392959	0.3153938228045661	0.4863254931615089	F	F	F
0.1121104352761861	0.1862923125396918	0.4862169103188876	F	F	F
0.0164653504910319	0.8169379209085434	0.5170864510602016	F	F	F
0.7737086930159478	0.4642121896258828	0.5098542901532497	F	F	F
0.3547568199701061	0.5398845750144545	0.4913055491984935	F	F	F
0.8548352112812623	0.9612879754852131	0.4913474116743402	F	F	F
0.2736558171006749	0.0367285287095171	0.5095842622449496	F	F	F
0.4364578605973435	0.0348585244096000	0.4598389770138454	F	F	F
0.6931547229194095	0.9653791778681509	0.5438751113830449	F	F	F
0.1930960752500894	0.5368671613790212	0.5435284188581946	F	F	F
0.9363025789852344	0.4660265976351923	0.4598071447971463	F	F	F
0.3719371349292804	0.8239217448608186	0.5808364235738035	T	T	T

0.1565922396629019	0.1913214662675018	0.6616133259761607	T	T	T
0.6536283382218476	0.3553761411512649	0.6542170282048018	T	T	T
0.8762417691711720	0.6897472453980771	0.5811678297063840	T	T	T
0.2237850529307563	0.6878750784214064	0.6415594977354367	T	T	T
0.3194526028851228	0.3215420311802185	0.6088485641132755	T	T	T
0.8176761654114774	0.1930354813164465	0.6063805036437421	T	T	T
0.7185736321041410	0.8303828154171222	0.6377855123091012	T	T	T
0.4849630834469247	0.4796357183745238	0.6245257083191551	T	T	T
0.0619542719298846	0.5408317846533918	0.6099947915749037	T	T	T
0.5623567254445980	0.9603219411904430	0.6102827879783077	T	T	T
0.9788966656909118	0.0388923350899135	0.6337108941523378	T	T	T
0.1448954601339625	0.0359980523104066	0.5797857947537797	T	T	T
0.4064942794688169	0.9660186862026797	0.6630114644565538	T	T	T
0.9027953804310165	0.5487527259160654	0.6637302650640952	T	T	T
0.6437554423694850	0.4940643382964844	0.5753978913298793	T	T	T
0.0689864051920905	0.6886117696751742	0.6990874881967678	T	T	T
0.3811771686547795	0.4612764331256020	0.7017398388628238	T	T	T
0.8458887924907337	0.0561635875219873	0.7003932076493098	T	T	T
0.5663496493230347	0.7269834047870076	0.6912762412369038	T	T	T
0.2780837511740519	0.9229141447259495	0.3013223712647137	T	T	T
0.5616586347583040	0.1746206096078375	0.3061056044459988	T	T	T
0.7700612251260746	0.5739945135385580	0.3013346994854088	T	T	T
0.0321222601733691	0.3148034611178692	0.2998726238138206	T	T	T
0.0027640280240898	0.6307497806376156	0.6929447133650544	T	T	T
0.3817610262111525	0.2721638984869195	0.6952551888734796	T	T	T
0.8651570342808046	0.2377678561680452	0.6953883123217640	T	T	T
0.6437693611824201	0.9302607936833593	0.7196686648973101	T	T	T
0.1062095632416882	0.5280122304807775	0.6984553937097434	T	T	T
0.4473022888379425	0.5072259230833774	0.7082427276341219	T	T	T

0.7790188956266809	0.0598670827833468	0.7152391612841906	T	T	T
0.5157341096853931	0.8551318787462105	0.6851611979826355	T	T	T
0.2243599413817277	0.9674361397175908	0.2823995626440793	T	T	T
0.2670489115551707	0.7384531376858611	0.3112428908856666	T	T	T
0.5185228410799622	0.0251733670194703	0.3071106385375597	T	T	T
0.6250049829802806	0.0992653023738398	0.3164817046599643	T	T	T
0.7587890914389696	0.7561482084846476	0.3131089889392660	T	T	T
0.7145530369692004	0.5352943969808973	0.2831861132740075	T	T	T
0.0238314700753222	0.4968087918281106	0.3098442482067599	T	T	T
0.9736688504570387	0.2741678187299540	0.2841476948547813	T	T	T
0.6592050281344348	0.2245827493630056	0.7126712395068661	T	T	T
0.6038266875967040	0.6379119651380055	0.6320608931960190	T	T	T
0.6487817750305567	0.6455289705310605	0.5195024736345744	F	F	F
0.6852019031743415	0.8704958410544240	0.3983752658669379	T	T	T

Ti O H Co

1.0000000000000000

14.2453041077000009 0.0000000000000000 0.0000000000000000

0.0000000000000000 5.1680002212999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 29.4789562224999990

Ti O H Co

21 57 17 3

Selective dynamics

Direct

0.0216741678505522	0.1119014340844360	0.3677714156994784	T	T	T
0.1853234307281535	0.6333087784983717	0.3959511108658760	T	T	T
0.5234264302590522	0.3954588080414758	0.3660905426243773	T	T	T
0.7658012754771722	0.3480249672616654	0.3662092867001477	T	T	T
0.9353492103211482	0.6370688963547744	0.3969915264965821	T	T	T



0.4414822216784703 0.8627518203684751 0.3983149869965424 T T T  
0.2735035510467173 0.1548569876716338 0.3642961023137106 T T T  
0.7342005810289152 0.1367530326270341 0.4848529224897646 F F F  
0.3956158154875027 0.8683481241609385 0.5172283169192724 F F F  
0.8953822014665107 0.6325289816178099 0.5172296942882255 F F F  
0.2344372928950307 0.3634625181788707 0.4844606095791164 F F F  
0.4815241771643173 0.3615968561732217 0.4834047030315531 F F F  
0.1487325421792534 0.8563983739423122 0.5193773182996253 F F F  
0.9814354254124780 0.1396032612863678 0.4834948480823442 F F F  
0.4485655267559087 0.1470453256564563 0.6051400908276983 T T T  
0.1056104831025204 0.9006038262103609 0.6384874178380124 T T T  
0.9414965438157001 0.3754617800672109 0.6060035288328299 T T T  
0.1831270839665841 0.3709005468877548 0.6049416172409204 T T T  
0.3539617986103795 0.6440751190976003 0.6349903609358495 T T T  
0.8528144278398739 0.8569824257840181 0.6375163701262065 T T T  
0.6881959746115555 0.1458138461117065 0.5980732992485566 T T T  
0.6089807885082287 -0.0616017681090038 0.7161275873334529 T T T  
0.9681779554500040 0.8215795259042870 0.3418569185231562 T T T  
0.7469182474497102 0.1707562670003686 0.4209494907625045 T T T  
0.2508070320015321 0.3128201889443872 0.4212050787086585 T T T  
0.4725143995381429 0.6867998122244450 0.3418798691317264 T T T  
0.8034012635000133 0.6886600224422909 0.3967746269368235 T T T  
0.8995391000564779 0.3188466587083946 0.3648384826659442 T T T  
0.4075741524359543 0.1805683836935493 0.3632189547623670 T T T  
0.3091407406845424 0.8151507419063120 0.3960914412112914 T T T  
0.0650285993612637 0.4644630995507626 0.3897760283170310 T T T  
0.6468945891708912 0.5430957576497013 0.3729068552374202 T T T  
0.1469388540440257 0.9664535728351416 0.3690457440721570 T T T  
0.5709945320458263 0.0315757782939306 0.3940258144578783 T T T

0.7206420790060916	0.0327786478331436	0.3401540185979097	T	T	T
0.9842018884745448	0.9659098298812999	0.4237884968166126	T	T	T
0.4835326146752312	0.5319878207651588	0.4235507147887106	T	T	T
0.2296192050546953	0.4589576065675054	0.3394040774574095	T	T	T
0.6690919997630900	0.8170932275262288	0.4621108699766978	F	F	F
0.4563443067348629	0.1856957460417874	0.5415381954083784	F	F	F
0.9563715435325619	0.3157762323396867	0.5415514049333012	F	F	F
0.1684768759925106	0.6845410757490313	0.4614047933963619	F	F	F
0.5163401794135183	0.6840621747006708	0.5172222351935218	F	F	F
0.6122121268392959	0.3153938228045661	0.4863254931615089	F	F	F
0.1121104352761861	0.1862923125396918	0.4862169103188876	F	F	F
0.0164653504910319	0.8169379209085434	0.5170864510602016	F	F	F
0.7737086930159478	0.4642121896258828	0.5098542901532497	F	F	F
0.3547568199701061	0.5398845750144545	0.4913055491984935	F	F	F
0.8548352112812623	0.9612879754852131	0.4913474116743402	F	F	F
0.2736558171006749	0.0367285287095171	0.5095842622449496	F	F	F
0.4364578605973435	0.0348585244096000	0.4598389770138454	F	F	F
0.6931547229194095	0.9653791778681509	0.5438751113830449	F	F	F
0.1930960752500894	0.5368671613790212	0.5435284188581946	F	F	F
0.9363025789852344	0.4660265976351923	0.4598071447971463	F	F	F
0.3726880061050528	0.8264316231392035	0.5820937052629731	T	T	T
0.1553978665562374	0.1941797054821299	0.6617773735598720	T	T	T
0.6626106416507208	0.3423325689929735	0.6587088390181737	T	T	T
0.8755723431125292	0.6927006485464140	0.5814372394317050	T	T	T
0.2227924873883093	0.6916539383263460	0.6406234570509707	T	T	T
0.3194316093378999	0.3151003934499387	0.6101082991823578	T	T	T
0.8179025545963873	0.1978457599592143	0.6047102726363491	T	T	T
0.7185614025151738	0.8338078618821309	0.6380533966565647	T	T	T
0.4853147024305361	0.4723763378352087	0.6294547510259635	T	T	T

0.0613373570569825	0.5437785786763449	0.6098431249185854	T	T	T
0.5623409320569863	0.9666517576861712	0.6106797002163165	T	T	T
0.9772875248096350	0.0472086120093167	0.6356754995625997	T	T	T
0.1427606187939672	0.0388480293584323	0.5800742564910569	T	T	T
0.4093636317942490	0.9562803164723088	0.6664413305138150	T	T	T
0.9032788635942129	0.5624782758708068	0.6643278291923747	T	T	T
0.6412323613795256	0.4930690948434460	0.5771910399101788	T	T	T
0.0682679006729231	0.6873694976360309	0.6988400467636912	T	T	T
0.3627932321079166	0.4441394537903937	0.7023174666102688	T	T	T
0.8245768592707798	0.1156552195225068	0.6972995697371176	T	T	T
0.5632057744919597	0.7260116968643037	0.6928585321242484	T	T	T
0.2768457122253496	0.9244921871627869	0.3011028335103942	T	T	T
0.5628034542144393	0.1787941122766787	0.3053672484754150	T	T	T
0.7688322236789593	0.5749541745600326	0.3015429286981134	T	T	T
0.0325429638387974	0.3135833842287569	0.2997264779119237	T	T	T
0.0020488905873055	0.6301782200525864	0.6912148676565245	T	T	T
0.3695811687287121	0.2567361215437734	0.6947782929162702	T	T	T
0.8690437543463276	0.2632747556250100	0.6948052283769068	T	T	T
0.1058147359862646	0.5272584763544461	0.6974590238225130	T	T	T
0.4227298344697176	0.4930524749743347	0.7160302793577916	T	T	T
0.7654304803219296	0.2024666372395168	0.6875243993296478	T	T	T
0.4695561459545922	0.8864456561281436	0.6803268027480284	T	T	T
0.2212811043956922	0.9690161702904034	0.2834511964393550	T	T	T
0.2668944058049158	0.7397161691844497	0.3110021294011946	T	T	T
0.5188626829340667	0.0315207095562157	0.3055709753376438	T	T	T
0.6253273264166400	0.1003395481248790	0.3161291671728018	T	T	T
0.7580082745347501	0.7572156483231719	0.3133981635478593	T	T	T
0.7122681272015241	0.5358614656004641	0.2841858866726029	T	T	T
0.0259359938534905	0.4960775998775942	0.3095760300647386	T	T	T

0.9726903407135546	0.2749295474644337	0.2850933920365539	T	T	T
0.6171148103481557	0.2477961349089934	0.6776122457991071	T	T	T
0.6728284431705212	-0.1295675525216427	0.7202925813149779	T	T	T
0.6062807355149390	0.6439867919546475	0.6327508306519859	T	T	T
0.6487817750305567	0.6455289705310605	0.5195024736345744	F	F	F
0.6854718521080829	0.8708953304174546	0.3988772492148969	T	T	T

Ti O H Co

1.0000000000000000

14.2453041077000009 0.0000000000000000 0.0000000000000000

0.0000000000000000 5.1680002212999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 29.4789562224999990

Ti O H Co

21 57 16 3

Selective dynamics

Direct

0.0224662839712136	0.1110649168110952	0.3676651659590967	T	T	T
0.1862198779071542	0.6334117718022596	0.3960228220512397	T	T	T
0.5243980637597243	0.3944382999827607	0.3661925978941401	T	T	T
0.7669987668377156	0.3474344547871268	0.3661728572689391	T	T	T
0.9365462225054945	0.6362316274899510	0.3970525183899746	T	T	T
0.4425200937687740	0.8628023204947374	0.3982315481070865	T	T	T
0.2742374202742538	0.1547229499035422	0.3643282792380970	T	T	T
0.7342005810289152	0.1367530326270341	0.4848529224897646	F	F	F
0.3956158154875027	0.8683481241609385	0.5172283169192724	F	F	F
0.8953822014665107	0.6325289816178099	0.5172296942882255	F	F	F
0.2344372928950307	0.3634625181788707	0.4844606095791164	F	F	F
0.4815241771643173	0.3615968561732217	0.4834047030315531	F	F	F
0.1487325421792534	0.8563983739423122	0.5193773182996253	F	F	F

0.9814354254124780 0.1396032612863678 0.4834948480823442 F F F  
0.4495818580970472 0.1505348588219784 0.6050769415593474 T T T  
0.1058661308020392 0.9000535522381075 0.6383674435488841 T T T  
0.9418621092319831 0.3742953511353861 0.6059776362549644 T T T  
0.1833053607923725 0.3712508659878293 0.6050076814486430 T T T  
0.3546120034956047 0.6451640738892582 0.6349855650504053 T T T  
0.8532831568792012 0.8547477159879979 0.6380215396939616 T T T  
0.6893825821100615 0.1478205341091272 0.5984301949043664 T T T  
0.5712074109688063 -0.0486954987831251 0.7105911743634673 T T T  
0.9693226213278548 0.8206060466862171 0.3417530676616019 T T T  
0.7476742482494707 0.1686506832837179 0.4207582996552259 T T T  
0.2515186105961472 0.3128462749393379 0.4212437180713248 T T T  
0.4737571551752230 0.6865109259442636 0.3419533274265221 T T T  
0.8044370453471256 0.6876522998169919 0.3966314873490520 T T T  
0.9005182957078527 0.3179061959455387 0.3648064747941811 T T T  
0.4084999892670615 0.1807813105948783 0.3632911589466093 T T T  
0.3100876700737658 0.8148680168230070 0.3961374746152569 T T T  
0.0659126157786883 0.4640459397128220 0.3897978891230392 T T T  
0.6480627796286783 0.5431906207288354 0.3726311622555065 T T T  
0.1479519779356531 0.9662417842848493 0.3690072273565192 T T T  
0.5719374086250222 0.0314074101385933 0.3940686814056972 T T T  
0.7214422671460972 0.0322672768787873 0.3399329914023848 T T T  
0.9847412646023116 0.9655048259964312 0.4236919539632871 T T T  
0.4843903707650382 0.5318995494444327 0.4236307758310081 T T T  
0.2306680621662474 0.4587399247194866 0.3394186917571335 T T T  
0.6690919997630900 0.8170932275262288 0.4621108699766978 F F F  
0.4563443067348629 0.1856957460417874 0.5415381954083784 F F F  
0.9563715435325619 0.3157762323396867 0.5415514049333012 F F F  
0.1684768759925106 0.6845410757490313 0.4614047933963619 F F F

0.5163401794135183 0.6840621747006708 0.5172222351935218 F F F  
0.6122121268392959 0.3153938228045661 0.4863254931615089 F F F  
0.1121104352761861 0.1862923125396918 0.4862169103188876 F F F  
0.0164653504910319 0.8169379209085434 0.5170864510602016 F F F  
0.7737086930159478 0.4642121896258828 0.5098542901532497 F F F  
0.3547568199701061 0.5398845750144545 0.4913055491984935 F F F  
0.8548352112812623 0.9612879754852131 0.4913474116743402 F F F  
0.2736558171006749 0.0367285287095171 0.5095842622449496 F F F  
0.4364578605973435 0.0348585244096000 0.4598389770138454 F F F  
0.6931547229194095 0.9653791778681509 0.5438751113830449 F F F  
0.1930960752500894 0.5368671613790212 0.5435284188581946 F F F  
0.9363025789852344 0.4660265976351923 0.4598071447971463 F F F  
0.3738140287325136 0.8296031139806583 0.5823597286086356 T T T  
0.1567332648153079 0.1933153694355906 0.6616173335141640 T T T  
0.6614271210291928 0.3375138748070830 0.6585952047177213 T T T  
0.8762176016951038 0.6916444337342195 0.5813807119581860 T T T  
0.2231648157169559 0.6915838128414029 0.6403439745382259 T T T  
0.3202290333728952 0.3208566135690892 0.6091615375846675 T T T  
0.8188608491391450 0.1953439111820169 0.6047327006815313 T T T  
0.7198325271021695 0.8338364966342143 0.6380607630197656 T T T  
0.4851522298911012 0.4743409131315344 0.6303628783337175 T T T  
0.0618001124992335 0.5434999123358809 0.6098085073698404 T T T  
0.5617705509158172 0.9659368663320100 0.6122052781009893 T T T  
0.9783406064094428 0.0447643408004439 0.6351760831660089 T T T  
0.1432498795417388 0.0387632978865137 0.5798970166321488 T T T  
0.4022195236205159 0.9713624966029368 0.6667545794106423 T T T  
0.9029812120250146 0.5561718827985859 0.6641103517248246 T T T  
0.6431495387586507 0.4904499366427343 0.5770567864343753 T T T  
0.0687546042339331 0.6870090673872427 0.6988188183561200 T T T

0.3556570451789800	0.4495600618678573	0.7023068883256915	T	T	T
0.8349915352514946	0.1018871309064384	0.6983209514603969	T	T	T
0.5790402070536257	0.7125984201975322	0.6954998397687289	T	T	T
0.2788216563129931	0.9236354095562693	0.3012496243656044	T	T	T
0.5634824199052045	0.1791937908544937	0.3052550064788805	T	T	T
0.7705312644604665	0.5736546360539738	0.3013821511514803	T	T	T
0.0334235165293580	0.3137729946287782	0.2997831156459940	T	T	T
0.0025254065116154	0.6291750749336092	0.6918075426490474	T	T	T
0.3573992813675885	0.2623422233437934	0.6937113176580720	T	T	T
0.8654935931433628	0.2721603075559744	0.6913492819436922	T	T	T
0.1062718323381734	0.5268588071857908	0.6976364285776683	T	T	T
0.4151592644415132	0.4816404474217701	0.7177132891043625	T	T	T
0.7679973458624270	0.1469207231815659	0.6983045059699527	T	T	T
0.4582469198792675	0.9602704169842845	0.6863841102384500	T	T	T
0.2239921622784432	0.9680183332724939	0.2830634187587042	T	T	T
0.2684740695016974	0.7390411016456240	0.3111478854788274	T	T	T
0.5195600397463851	0.0319372898790497	0.3053465533331229	T	T	T
0.6259749760816558	0.1004682180387162	0.3159493036207570	T	T	T
0.7596357228388133	0.7559346770311534	0.3131007188519547	T	T	T
0.7142552533450854	0.5345302279064772	0.2838141156790715	T	T	T
0.0264714694978322	0.4962359974665644	0.3096335799953104	T	T	T
0.9738713679351670	0.2747008538811447	0.2849078659722983	T	T	T
0.6142764046964917	0.2360409013042115	0.6756516145776681	T	T	T
0.6072523367065736	0.6447644921908116	0.6341734878905202	T	T	T
0.6487817750305567	0.6455289705310605	0.5195024736345744	F	F	F
0.6869842416528019	0.8700529672244223	0.3981256226061474	T	T	T

Ti O H Co

1.000000000000000

14.2453041077000009 0.0000000000000000 0.0000000000000000  
0.0000000000000000 5.1680002212999998 0.0000000000000000  
0.0000000000000000 0.0000000000000000 29.4789562224999990

Ti O H Co

21 57 15 3

Selective dynamics

Direct

0.0215363927666328 0.1092507010236356 0.3673457374834712 T T T  
0.1844183275897141 0.6326806633703878 0.3964520696379371 T T T  
0.5223595576804109 0.4010156363949240 0.3654470449015386 T T T  
0.7663817357591142 0.3500969391866882 0.3661147511537800 T T T  
0.9358968323716593 0.6356468757704771 0.3974599385377121 T T T  
0.4394153432449856 0.8646394660176588 0.3993791551181152 T T T  
0.2730421390373912 0.1568958053790000 0.3639288398327417 T T T  
0.7342005810289152 0.1367530326270341 0.4848529224897646 F F F  
0.3956158154875027 0.8683481241609385 0.5172283169192724 F F F  
0.8953822014665107 0.6325289816178099 0.5172296942882255 F F F  
0.2344372928950307 0.3634625181788707 0.4844606095791164 F F F  
0.4815241771643173 0.3615968561732217 0.4834047030315531 F F F  
0.1487325421792534 0.8563983739423122 0.5193773182996253 F F F  
0.9814354254124780 0.1396032612863678 0.4834948480823442 F F F  
0.4393998421610934 0.1496457494733656 0.6063819164267750 T T T  
0.1081981048448494 0.8984254901448649 0.6379783144334964 T T T  
0.9439973332275459 0.3745593619076948 0.6063970230755175 T T T  
0.1865329480416887 0.3721136100282888 0.6053235501858292 T T T  
0.3588137032569514 0.6664623030184874 0.6379527238679624 T T T  
0.8540466288125201 0.8557895617932382 0.6373052009470218 T T T  
0.6892692921393541 0.1448298611867496 0.5989359185482936 T T T  
0.5889471238193460 0.9483554706100884 0.7119050820228805 T T T



0.9687278986884386	0.8192235336509378	0.3416344843539595	T	T	T
0.7468677381536579	0.1693705214661143	0.4206463965459731	T	T	T
0.2505376312192926	0.3131001564607300	0.4209041006340601	T	T	T
0.4731337667080981	0.6925208401526131	0.3416617424495759	T	T	T
0.8037430680353190	0.6878920842048737	0.3966450472655035	T	T	T
0.8996165191865042	0.3178603608352922	0.3648121800534474	T	T	T
0.4078920755286368	0.1814311834529511	0.3636210628806870	T	T	T
0.3092523023315938	0.8141477158295684	0.3961856072760103	T	T	T
0.0651111942304629	0.4637094201062776	0.3897502763932226	T	T	T
0.6471019997404195	0.5446924067107285	0.3727042900139917	T	T	T
0.1473072775593199	0.9662959526043584	0.3689487140789680	T	T	T
0.5724199281651784	0.0296993779854185	0.3940716779415403	T	T	T
0.7206011811555167	0.0329550378196910	0.3401312757635910	T	T	T
0.9841744873643485	0.9649984464544474	0.4234988815314761	T	T	T
0.4837674457842384	0.5327666116074600	0.4232552512773778	T	T	T
0.2300131989575316	0.4596893983474866	0.3390896197290327	T	T	T
0.6690919997630900	0.8170932275262288	0.4621108699766978	F	F	F
0.4563443067348629	0.1856957460417874	0.5415381954083784	F	F	F
0.9563715435325619	0.3157762323396867	0.5415514049333012	F	F	F
0.1684768759925106	0.6845410757490313	0.4614047933963619	F	F	F
0.5163401794135183	0.6840621747006708	0.5172222351935218	F	F	F
0.6122121268392959	0.3153938228045661	0.4863254931615089	F	F	F
0.1121104352761861	0.1862923125396918	0.4862169103188876	F	F	F
0.0164653504910319	0.8169379209085434	0.5170864510602016	F	F	F
0.7737086930159478	0.4642121896258828	0.5098542901532497	F	F	F
0.3547568199701061	0.5398845750144545	0.4913055491984935	F	F	F
0.8548352112812623	0.9612879754852131	0.4913474116743402	F	F	F
0.2736558171006749	0.0367285287095171	0.5095842622449496	F	F	F
0.4364578605973435	0.0348585244096000	0.4598389770138454	F	F	F

0.6931547229194095 0.9653791778681509 0.5438751113830449 F F F  
0.1930960752500894 0.5368671613790212 0.5435284188581946 F F F  
0.9363025789852344 0.4660265976351923 0.4598071447971463 F F F  
0.3746620471495173 0.8200666985561209 0.5809587025711915 T T T  
0.1563936370722467 0.1934419643330338 0.6615199666144360 T T T  
0.6565334814521274 0.3503988918464651 0.6574242169098559 T T T  
0.8754416285873570 0.6925249297227623 0.5810031892268774 T T T  
0.2228717483393183 0.6894289322286172 0.6404499070904526 T T T  
0.3185426342383023 0.3210205135484132 0.6075652575676256 T T T  
0.8174615867378706 0.1982500551372875 0.6049857236548916 T T T  
0.7181225083684351 0.8376675357756133 0.6377228989138533 T T T  
0.4844831466959930 0.4765107332016394 0.6292079220955269 T T T  
0.0608499419978689 0.5439503757299687 0.6098307156094095 T T T  
0.5620957400284231 0.9678659521565466 0.6113176827605045 T T T  
0.9773874462196843 0.0443262048726947 0.6347770875583003 T T T  
0.1433085839126109 0.0377606809996314 0.5795943933600484 T T T  
0.4002369861925799 0.9690341407906057 0.6631557832298156 T T T  
0.9014499431178398 0.5564707193020416 0.6639413463628336 T T T  
0.6426585658537013 0.4950436473885922 0.5760808632035399 T T T  
0.0686153736064761 0.6882889274792869 0.6987941299677713 T T T  
0.3578818620876706 0.4384727338628504 0.7014829913331894 T T T  
0.8354216540437497 0.0979599255984270 0.6985992591983720 T T T  
0.5709502038352543 0.7273353297045922 0.6943525359743815 T T T  
0.2780465591299551 0.9234575556971886 0.3012545840765761 T T T  
0.5620108697976945 0.1771584520874965 0.3058363130368107 T T T  
0.7696222518673842 0.5754870980056246 0.3014054499350055 T T T  
0.0324809308849752 0.3148439319811480 0.2997862060881790 T T T  
0.0023538371357045 0.6318661332908480 0.6920502883640265 T T T  
0.3662526623541583 0.2520369123308722 0.6926639123623867 T T T

0.8612270421773848	0.2732711938512618	0.6909483677961659	T	T	T
0.1056513785811249	0.5272861837251105	0.6975901035070596	T	T	T
0.4134844795099407	0.4832276594220495	0.7191122539033465	T	T	T
0.7677228932946767	0.1272272564585533	0.7011348912630092	T	T	T
0.2236420034476779	0.9677755348342757	0.2827770370015187	T	T	T
0.2672916881646852	0.7390021803689339	0.3112675367716218	T	T	T
0.5186686312966943	0.0282807724852276	0.3067665366547035	T	T	T
0.6250574900219642	0.1010927826155178	0.3164101847390483	T	T	T
0.7586204428961263	0.7577170938233997	0.3132362263023210	T	T	T
0.7135347484605390	0.5367062237983090	0.2836783493698024	T	T	T
0.0251067805454463	0.4970084632341404	0.3098035538827750	T	T	T
0.9732791496514661	0.2757028674997928	0.2845992176797242	T	T	T
0.6100710892666809	0.2518328609373164	0.6752365171064243	T	T	T
0.6030160902671797	0.6521029813404355	0.6320597693325483	T	T	T
0.6487817750305567	0.6455289705310605	0.5195024736345744	F	F	F
0.6854652053101973	0.8725158181329847	0.3984182143366664	T	T	T

Ti O H Co

1.000000000000000

14.2453041077000009 0.0000000000000000 0.0000000000000000

0.0000000000000000 5.1680002212999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 29.4789562224999990

Ti O H Co

21 55 15 3

Selective dynamics

Direct

0.0221519741757002	0.1127349967540753	0.3678535044776058	T	T	T
0.1861986826678043	0.6342317065902530	0.3960458867703438	T	T	T
0.5234107905996911	0.3959074560286874	0.3661658948691584	T	T	T

0.7661388925436964	0.3489644008044631	0.3664390197993763	T	T	T
0.9361054512405450	0.6373493728077562	0.3968112830533210	T	T	T
0.4421802865698256	0.8638534498575335	0.3983989992181974	T	T	T
0.2737236181776889	0.1552680412278014	0.3642270363922722	T	T	T
0.7342005810289152	0.1367530326270341	0.4848529224897646	F	F	F
0.3956158154875027	0.8683481241609385	0.5172283169192724	F	F	F
0.8953822014665107	0.6325289816178099	0.5172296942882255	F	F	F
0.2344372928950307	0.3634625181788707	0.4844606095791164	F	F	F
0.4815241771643173	0.3615968561732217	0.4834047030315531	F	F	F
0.1487325421792534	0.8563983739423122	0.5193773182996253	F	F	F
0.9814354254124780	0.1396032612863678	0.4834948480823442	F	F	F
0.4413538226547097	0.1456784752485689	0.6058659582076902	T	T	T
0.1100343507546685	0.8987873314554012	0.6382991889427011	T	T	T
0.9449695125155819	0.3737631852619833	0.6060879658015329	T	T	T
0.1881708609257778	0.3722280966740960	0.6049788871809492	T	T	T
0.3603286242111891	0.6667272994974353	0.6385057856268019	T	T	T
0.8564801613213809	0.8537083153240560	0.6378460358859601	T	T	T
0.6896752602277337	0.1315890374952517	0.5996252867563356	T	T	T
0.9682992479613111	0.8222790327141859	0.3418578900196931	T	T	T
0.7470501325485696	0.1713096827781094	0.4211258241847907	T	T	T
0.2510103002903007	0.3132422640321116	0.4211354947490492	T	T	T
0.4727021968110420	0.6868299385600333	0.3418627016325143	T	T	T
0.8035522070873129	0.6876711891606789	0.3969069953344470	T	T	T
0.8996636205511903	0.3191595334765605	0.3646921799274609	T	T	T
0.4077595522799057	0.1808815408495449	0.3630654680216791	T	T	T
0.3092288622478928	0.8157786859139033	0.3960495071764485	T	T	T
0.0650817204774870	0.4647183183883601	0.3897602120610550	T	T	T
0.6470105857941243	0.5435697429789103	0.3732498780269111	T	T	T
0.1470834083714475	0.9669487431254293	0.3690206181296091	T	T	T

0.5707879924085842 0.0321802413197199 0.3941646090575575 T T T  
0.7205264834173614 0.0313535194801463 0.3407944264950724 T T T  
0.9842818859652983 0.9661351340694405 0.4237749403684185 T T T  
0.4835718392516983 0.5327556988297665 0.4235588793819560 T T T  
0.2297045444919405 0.4593230148720189 0.3393644525377030 T T T  
0.6690919997630900 0.8170932275262288 0.4621108699766978 F F F  
0.4563443067348629 0.1856957460417874 0.5415381954083784 F F F  
0.9563715435325619 0.3157762323396867 0.5415514049333012 F F F  
0.1684768759925106 0.6845410757490313 0.4614047933963619 F F F  
0.5163401794135183 0.6840621747006708 0.5172222351935218 F F F  
0.6122121268392959 0.3153938228045661 0.4863254931615089 F F F  
0.1121104352761861 0.1862923125396918 0.4862169103188876 F F F  
0.0164653504910319 0.8169379209085434 0.5170864510602016 F F F  
0.7737086930159478 0.4642121896258828 0.5098542901532497 F F F  
0.3547568199701061 0.5398845750144545 0.4913055491984935 F F F  
0.8548352112812623 0.9612879754852131 0.4913474116743402 F F F  
0.2736558171006749 0.0367285287095171 0.5095842622449496 F F F  
0.4364578605973435 0.0348585244096000 0.4598389770138454 F F F  
0.6931547229194095 0.9653791778681509 0.5438751113830449 F F F  
0.1930960752500894 0.5368671613790212 0.5435284188581946 F F F  
0.9363025789852344 0.4660265976351923 0.4598071447971463 F F F  
0.3753857136958848 0.8214704540683152 0.5818404505141958 T T T  
0.1569426794238967 0.1946090069786711 0.6617337414867642 T T T  
0.6537647132897643 0.3452990346452172 0.6585954882247018 T T T  
0.8754599445104470 0.6912408179499578 0.5817568285067483 T T T  
0.2240607983074299 0.6902649953708924 0.6404747604310969 T T T  
0.3201128714467040 0.3203509102446850 0.6082466247198155 T T T  
0.8166911931121669 0.1979361183616610 0.6061241836080524 T T T  
0.7164682307678242 0.8256611641863277 0.6379597644276961 T T T

0.4874024381870582 0.4771965184634427 0.6310026067159160 T T T  
0.0613016593310843 0.5426303555615132 0.6100871511707734 T T T  
0.5615058193538920 0.9660139290853451 0.6114809889951480 T T T  
0.9773644024831325 0.0431868292698718 0.6354005819754855 T T T  
0.1437347706098335 0.0385234809980926 0.5799471752341967 T T T  
0.4031076530391335 0.9657101591935980 0.6644982857169978 T T T  
0.9030134894699737 0.5568719942750173 0.6647323303112059 T T T  
0.6414663230798316 0.4847731894674327 0.5745444727201316 T T T  
0.0706163042808021 0.6853487440026262 0.6989513637855805 T T T  
0.3544559475859090 0.4269464208937903 0.7009276520378441 T T T  
0.8292237732066309 0.1037960599144713 0.6981152857252622 T T T  
0.2768998108069603 0.9245509943327233 0.3010523476011670 T T T  
0.5638056038716781 0.1804695532756619 0.3053495181381420 T T T  
0.7675875196549917 0.5738463085838565 0.3016311158062985 T T T  
0.0329319164095795 0.3129256050181848 0.2996602574308911 T T T  
0.0042296548653501 0.6299029626582056 0.6921871806022478 T T T  
0.3661392484011963 0.2415585735245461 0.6916018709322131 T T T  
0.8623619561327313 0.2707963273230312 0.6915559606047005 T T T  
0.1073983649120763 0.5239126813637639 0.6968709807805092 T T T  
0.4031614218295809 0.4704953727094957 0.7227445192680021 T T T  
0.7629884996328885 0.1546076557569899 0.6952460801598620 T T T  
0.2211143700388186 0.9687542293815469 0.2835391995663299 T T T  
0.2670910562425085 0.7398210719082224 0.3110165836123662 T T T  
0.5193586481569125 0.0344699225924325 0.3051468994282083 T T T  
0.6257470752193640 0.1001619420301316 0.3165212177712926 T T T  
0.7571056937155334 0.7560238477886363 0.3136009907597635 T T T  
0.7103892827715641 0.5345560666347973 0.2847760558771668 T T T  
0.0270357740272233 0.4956286265627107 0.3094419107186928 T T T  
0.9726616283513952 0.2752557050733085 0.2853533296853423 T T T

0.5955598458202457	0.2611030054667731	0.6684803963378937	T	T	T
0.6065999198448256	0.6384097760515970	0.6260587323411436	T	T	T
0.6487817750305567	0.6455289705310605	0.5195024736345744	F	F	F
0.6856375892369475	0.8701973553796798	0.3991947779419791	T	T	T

Ti O H Co

1.0000000000000000

14.2453041077000009 0.0000000000000000 0.0000000000000000

0.0000000000000000 5.1680002212999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 29.4789562224999990

Ti O H Co

21 55 14 3

Selective dynamics

Direct

0.0231833123856332	0.1134762996702526	0.3678421629632800	T	T	T
0.1884105319788609	0.6362163702094569	0.3961307952625481	T	T	T
0.5242366854400090	0.3939212935396393	0.3667151707543574	T	T	T
0.7675594234602734	0.3497721496446328	0.3666654751622279	T	T	T
0.9383712267574540	0.6369099264279544	0.3966677588516109	T	T	T
0.4446531675803495	0.8659442405392188	0.3979558891639616	T	T	T
0.2743613876075385	0.1555827032726921	0.3642146915862288	T	T	T
0.7342005810289152	0.1367530326270341	0.4848529224897646	F	F	F
0.3956158154875027	0.8683481241609385	0.5172283169192724	F	F	F
0.8953822014665107	0.6325289816178099	0.5172296942882255	F	F	F
0.2344372928950307	0.3634625181788707	0.4844606095791164	F	F	F
0.4815241771643173	0.3615968561732217	0.4834047030315531	F	F	F
0.1487325421792534	0.8563983739423122	0.5193773182996253	F	F	F
0.9814354254124780	0.1396032612863678	0.4834948480823442	F	F	F
0.4385485395638303	0.1493666100462888	0.6059843064872323	T	T	T

0.1090472776803373	0.8976436521620933	0.6383229615523121	T	T	T
0.9433133705393706	0.3718097631556192	0.6062444371419485	T	T	T
0.1858473358685739	0.3721588967819150	0.6050423942234918	T	T	T
0.3593562208915968	0.6669208870830511	0.6380092888134782	T	T	T
0.8553307218900289	0.8534233194878995	0.6372627450486148	T	T	T
0.6869111114830726	0.1397009659708058	0.6006032663709620	T	T	T
0.9692292055261071	0.8223978812540903	0.3417918835696721	T	T	T
0.7477770118915700	0.1695881455250279	0.4211087048624361	T	T	T
0.2518468688591725	0.3138846969484824	0.4211134969834236	T	T	T
0.4738444428704504	0.6853945680092857	0.3420257876902660	T	T	T
0.8044867924966125	0.6846998830948141	0.3969886700455040	T	T	T
0.9004859295892396	0.3186667857363442	0.3643966588792022	T	T	T
0.4083876993601659	0.1819405206143696	0.3626781070332293	T	T	T
0.3099496517085732	0.8169296514203940	0.3959783149840001	T	T	T
0.0656331885009566	0.4646593749278084	0.3898411888034497	T	T	T
0.6479946876378863	0.5443571292033091	0.3737129678846269	T	T	T
0.1478061843272798	0.9676130647016871	0.3689599889774514	T	T	T
0.5707021244974456	0.0355865875279862	0.3944489100245827	T	T	T
0.7205708196950512	0.0280965333867145	0.3415407739323446	T	T	T
0.9847459423400866	0.9659938831587123	0.4236901878847215	T	T	T
0.4843067270998054	0.5344216607531584	0.4238003734477572	T	T	T
0.2301862465807629	0.4598233973829856	0.3393608636345462	T	T	T
0.6690919997630900	0.8170932275262288	0.4621108699766978	F	F	F
0.4563443067348629	0.1856957460417874	0.5415381954083784	F	F	F
0.9563715435325619	0.3157762323396867	0.5415514049333012	F	F	F
0.1684768759925106	0.6845410757490313	0.4614047933963619	F	F	F
0.5163401794135183	0.6840621747006708	0.5172222351935218	F	F	F
0.6122121268392959	0.3153938228045661	0.4863254931615089	F	F	F
0.1121104352761861	0.1862923125396918	0.4862169103188876	F	F	F



0.0164653504910319 0.8169379209085434 0.5170864510602016 F F F  
0.7737086930159478 0.4642121896258828 0.5098542901532497 F F F  
0.3547568199701061 0.5398845750144545 0.4913055491984935 F F F  
0.8548352112812623 0.9612879754852131 0.4913474116743402 F F F  
0.2736558171006749 0.0367285287095171 0.5095842622449496 F F F  
0.4364578605973435 0.0348585244096000 0.4598389770138454 F F F  
0.69315472229194095 0.9653791778681509 0.5438751113830449 F F F  
0.1930960752500894 0.5368671613790212 0.5435284188581946 F F F  
0.9363025789852344 0.4660265976351923 0.4598071447971463 F F F  
0.3728539298812629 0.8228542940137954 0.5813596181719306 T T T  
0.1560550869010706 0.1933571016645393 0.6617499666314647 T T T  
0.6528771785806662 0.3692389618222896 0.6552082729857261 T T T  
0.8748201067027451 0.6909606751701640 0.5813372731208405 T T T  
0.2229972685492999 0.6885863417763304 0.6406404602582891 T T T  
0.3187211088615081 0.3189560545801743 0.6080040945074754 T T T  
0.8159779854752486 0.1968882529422225 0.6062183714369896 T T T  
0.7173683455519118 0.8333915326293903 0.6384794956152310 T T T  
0.4839825421079502 0.4781442262237767 0.6285928260037753 T T T  
0.0604672385882145 0.5415894649183693 0.6099996080121195 T T T  
0.5611338635463536 0.9532055993443675 0.6125313698194692 T T T  
0.9771151063562270 0.0423093395660740 0.6348953188628592 T T T  
0.1432295056479091 0.0377119368131494 0.5799008598531979 T T T  
0.4026398231698379 0.9660556755871670 0.6638150275369974 T T T  
0.9014191783653697 0.5542514802027629 0.6642943837335304 T T T  
0.6401616514267047 0.4739217086286791 0.5729192458113659 T T T  
0.0688827110904161 0.6847723202170268 0.6988407573352883 T T T  
0.3573016625476932 0.4313577674694342 0.7011493344175602 T T T  
0.8348472998774507 0.0947257346996314 0.6992450492819928 T T T  
0.2776473815828261 0.9249702623432156 0.3009460697082250 T T T

0.5668183297481703	0.1884006655255144	0.3048724858921717	T	T	T
0.7662585431323733	0.5699748865932197	0.3016046888169614	T	T	T
0.0341836335344376	0.3122689636908988	0.2995873492172124	T	T	T
0.0024981303116224	0.6295827593777351	0.6920422987601478	T	T	T
0.3673142347944494	0.2457539298819042	0.6918140860585754	T	T	T
0.8599764823943172	0.2704736485848908	0.6912946028776041	T	T	T
0.1055640318777346	0.5231135792913801	0.6970252543402596	T	T	T
0.4104847578852822	0.4741396215185220	0.7204875923475770	T	T	T
0.7671804837891735	0.1212721531391297	0.7021542895109216	T	T	T
0.2218525800226070	0.9691749064371663	0.2834352564392205	T	T	T
0.2677973069982915	0.7402818427243381	0.3109081092538162	T	T	T
0.5209316678435502	0.0468293033517763	0.3028076334545809	T	T	T
0.6269289059808356	0.1012741418731752	0.3168572901162848	T	T	T
0.7561551099262025	0.7523395305251206	0.3135484111636174	T	T	T
0.7081841973212858	0.5293115164372363	0.2855237861845549	T	T	T
0.0283427944877423	0.4951773483180000	0.3092397300384006	T	T	T
0.9739944000569026	0.2743624586961052	0.2852208870104108	T	T	T
0.6063508836818162	0.6348067571364645	0.6287185660501248	T	T	T
0.6487817750305567	0.6455289705310605	0.5195024736345744	F	F	F
0.6871763702342381	0.8681362734941227	0.3992039322054461	T	T	T

Ti O Ti O Ti O

1.0000000000000000

14.2453041077000009 0.0000000000000000 0.0000000000000000

0.0000000000000000 5.1680002212999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 29.4789562224999990

Ti O H Co

21 56 16 3

Selective dynamics

## Direct

0.0214833785536923	0.1097001313613181	0.3675892937340928	T	T	T
0.1846359792307998	0.6325822985127546	0.3962736809013391	T	T	T
0.5226768661668889	0.3984084433526341	0.3655069429312054	T	T	T
0.7660703362822292	0.3469810176263557	0.3661580871054518	T	T	T
0.9355130227339046	0.6355424901665464	0.3972459308544835	T	T	T
0.4399832856590635	0.8627563163867976	0.3990831054034032	T	T	T
0.2732135551345701	0.1558873856025741	0.3640950444251927	T	T	T
0.7342005810289152	0.1367530326270341	0.4848529224897646	F	F	F
0.3956158154875027	0.8683481241609385	0.5172283169192724	F	F	F
0.8953822014665107	0.6325289816178099	0.5172296942882255	F	F	F
0.2344372928950307	0.3634625181788707	0.4844606095791164	F	F	F
0.4815241771643173	0.3615968561732217	0.4834047030315531	F	F	F
0.1487325421792534	0.8563983739423122	0.5193773182996253	F	F	F
0.9814354254124780	0.1396032612863678	0.4834948480823442	F	F	F
0.4451808620787467	0.1414623697321191	0.6055991490229180	T	T	T
0.1049877611872243	0.8957841832699793	0.6352599207422642	T	T	T
0.9410876370407111	0.3699780460299363	0.6066389966507428	T	T	T
0.1882938637298783	0.3711960711605656	0.6064151599063443	T	T	T
0.3587999146640210	0.6585694328019031	0.6365160912194044	T	T	T
0.8531681348014768	0.8444490190287741	0.6377238095711802	T	T	T
0.6874019807234503	0.1389846219218743	0.6007362212611795	T	T	T
0.9684452952048671	0.8198375472710160	0.3417242579196645	T	T	T
0.7470818067005054	0.1682543721752163	0.4205873345552914	T	T	T
0.2505781101157235	0.3128379696638976	0.4210050828628273	T	T	T
0.4726059991954866	0.6895493305748167	0.3416670044554296	T	T	T
0.8034406020850577	0.6868669312045832	0.3965860308300497	T	T	T
0.8997151148384697	0.3178705661698946	0.3647104655371918	T	T	T
0.4077792313184364	0.1798131063815235	0.3634444661764525	T	T	T

0.3091191391731697 0.8139931971874348 0.3962029161871729 T T T  
0.0650603605369369 0.4636534459714934 0.3897507180144305 T T T  
0.6469374444387882 0.5419954540014995 0.3725039299761738 T T T  
0.1471670325203842 0.9659951649099898 0.3689741465912466 T T T  
0.5720733931549148 0.0277658869213445 0.3939576368516762 T T T  
0.7207246075129964 0.0309821825654745 0.3399592064330960 T T T  
0.9841682086876217 0.9647244652557484 0.4236461138764343 T T T  
0.4835734522611677 0.5312938356414619 0.4232477485065831 T T T  
0.2299097715658397 0.4591145360142996 0.3392033145001366 T T T  
0.6690919997630900 0.8170932275262288 0.4621108699766978 F F F  
0.4563443067348629 0.1856957460417874 0.5415381954083784 F F F  
0.9563715435325619 0.3157762323396867 0.5415514049333012 F F F  
0.1684768759925106 0.6845410757490313 0.4614047933963619 F F F  
0.5163401794135183 0.6840621747006708 0.5172222351935218 F F F  
0.6122121268392959 0.3153938228045661 0.4863254931615089 F F F  
0.1121104352761861 0.1862923125396918 0.4862169103188876 F F F  
0.0164653504910319 0.8169379209085434 0.5170864510602016 F F F  
0.7737086930159478 0.4642121896258828 0.5098542901532497 F F F  
0.3547568199701061 0.5398845750144545 0.4913055491984935 F F F  
0.8548352112812623 0.9612879754852131 0.4913474116743402 F F F  
0.2736558171006749 0.0367285287095171 0.5095842622449496 F F F  
0.4364578605973435 0.0348585244096000 0.4598389770138454 F F F  
0.6931547229194095 0.9653791778681509 0.5438751113830449 F F F  
0.1930960752500894 0.5368671613790212 0.5435284188581946 F F F  
0.9363025789852344 0.4660265976351923 0.4598071447971463 F F F  
0.3729831583820037 0.8228266229705319 0.5811733428745824 T T T  
0.1544058013990681 0.1880427547055350 0.6617742331299181 T T T  
0.6530110380882741 0.3474773625369728 0.6542616983339264 T T T  
0.8759796413982311 0.6892743361794073 0.5811852142082455 T T T

0.2251714136741182 0.6906817481523623 0.6395609703432674 T T T  
0.3196202967616745 0.3128028764038900 0.6100412510441963 T T T  
0.8174491467463999 0.1912149129642945 0.6071852469192535 T T T  
0.7173844229432346 0.8277425930421163 0.6380694136543681 T T T  
0.4847887253973453 0.4743653394314855 0.6270968966203837 T T T  
0.0605744746901386 0.5427371248735307 0.6128173564079167 T T T  
0.5620267331985725 0.9617260224305785 0.6092211004956832 T T T  
0.9784239802774193 0.0364573689882202 0.6333929649384743 T T T  
0.1443227203604628 0.0397582201891618 0.5793180323825594 T T T  
0.4099936627116028 0.9518534521548346 0.6648337498315197 T T T  
0.8959785653550328 0.5440309564485251 0.6635905773503914 T T T  
0.6421846784527417 0.4898242885275593 0.5754783764997925 T T T  
0.0899017139949575 0.6936283563977893 0.7034536318186647 T T T  
0.3644519065184381 0.4304967235722849 0.7020044006950992 T T T  
0.8479606323284409 0.0766970143347483 0.7014332017176371 T T T  
0.5682276190345528 0.7642544183108303 0.6926575704294736 T T T  
0.2769025387705585 0.9239170577859090 0.3011039190677773 T T T  
0.5622660344553175 0.1746279904299556 0.3058581670319696 T T T  
0.7690283632161311 0.5729708190667702 0.3011954007957006 T T T  
0.0326725548746917 0.3138364605331149 0.2996712858129345 T T T  
0.0953509175742906 0.5110778299984855 0.6934618519475680 T T T  
0.3710970420034370 0.2452423133182195 0.6922662194047244 T T T  
0.9032435861331199 0.0301309724881318 0.7191367291424304 T T T  
0.6167202949253041 0.8962594361004499 0.6974436588195172 T T T  
0.1502270008411211 0.7286589900791444 0.7179197767435039 T T T  
0.4245380660850051 0.4722199855082300 0.7161535180283296 T T T  
0.8589239679995134 0.2608560544283280 0.6915228432342193 T T T  
0.5075626738541864 0.8624814567672592 0.6843438060118836 T T T  
0.2211871804888296 0.9683235892419100 0.2835515110144365 T T T

0.2668468660939581	0.7392678376018909	0.3111323682160075	T	T	T
0.5189276870457962	0.0257548719519676	0.3068665931214185	T	T	T
0.6254569343430044	0.0987250466780823	0.3164512245488703	T	T	T
0.7584301135011355	0.7552098139024123	0.3130645333558283	T	T	T
0.7120939738137333	0.5340807550666413	0.2841080167490520	T	T	T
0.0264187172917135	0.4959780519707051	0.3098052155721165	T	T	T
0.9725076728986857	0.2767652596696688	0.2852208890828104	T	T	T
0.6057569145354035	0.6308590014649799	0.6305723991600762	T	T	T
0.6487817750305567	0.6455289705310605	0.5195024736345744	F	F	F
0.6854891202752553	0.8698778793234960	0.3984340908304758	T	T	T

=====Co first layer structures=====

Ti O Ti O Ti O

1.0000000000000000

14.2453041077000009 0.0000000000000000 0.0000000000000000

0.0000000000000000 5.1680002212999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 29.4789562224999990

Ti O H Co Ti

21 57 18 1 2

Selective dynamics

Direct

0.0213740338551517	0.1072130200064282	0.3670344240447669	T	T	T
0.1846652110515387	0.6329091369570541	0.3965016728639330	T	T	T
0.5178773001431267	0.3954475321391078	0.3649136092902358	T	T	T
0.7696589323025346	0.3494150881560937	0.3653516931291593	T	T	T
0.9386101007402443	0.6329837406925753	0.3972443994680492	T	T	T
0.4383330235467768	0.8665782361633706	0.3982255800263241	T	T	T
0.2703050394453262	0.1571403915908518	0.3634640379307903	T	T	T
0.7342005810289152	0.1367530326270341	0.4848529224897646	F	F	F

0.3956158154875027 0.8683481241609385 0.5172283169192724 F F F  
0.8953822014665107 0.6325289816178099 0.5172296942882255 F F F  
0.2344372928950307 0.3634625181788707 0.4844606095791164 F F F  
0.4815241771643173 0.3615968561732217 0.4834047030315531 F F F  
0.1487325421792534 0.8563983739423122 0.5193773182996253 F F F  
0.9814354254124780 0.1396032612863678 0.4834948480823442 F F F  
0.4454068469298698 0.1392263761657409 0.6062361902535763 T T T  
0.1066584966129277 0.8941009562915473 0.6379627177172126 T T T  
0.9434098373858535 0.3677254691062229 0.6064894070112520 T T T  
0.1869880358923319 0.3656221144926782 0.6053264207106633 T T T  
0.3567031688849855 0.6555406689980200 0.6368202500207339 T T T  
0.8534125887686195 0.8451205341902599 0.6383646741250778 T T T  
0.6875299783682520 0.1419486152778262 0.6032915942176870 T T T  
0.6693839103266684 0.1142308906815739 0.7319171338999994 T T T  
0.9709249095242138 0.8149824532232796 0.3412335426140842 T T T  
0.7503098584738799 0.1859495699311293 0.4211828316048707 T T T  
0.2506497481740595 0.3135170567326099 0.4208814129931327 T T T  
0.4685425022347106 0.6880256768867028 0.3413712964289253 T T T  
0.8084240090469618 0.6893286533212650 0.3950008395613346 T T T  
0.9023496545390610 0.3130849455389862 0.3638893927948754 T T T  
0.4044793054688811 0.1821921797456330 0.3618658194955164 T T T  
0.3084407225075892 0.8164769839487896 0.3964078438603161 T T T  
0.0665266119593142 0.4592597172994290 0.3899153328621269 T T T  
0.6463522900924832 0.5394072063653736 0.3688571373098236 T T T  
0.1474040602446614 0.9644042294099388 0.3686022971384101 T T T  
0.5658782524399210 0.0391309453336183 0.3926754264301784 T T T  
0.7224655489725195 0.0494804248668551 0.3377958124393148 T T T  
0.9850836757924105 0.9633215754352368 0.4234981287893024 T T T  
0.4844265017122796 0.5345355776490048 0.4231893214706130 T T T

0.2288220270141637 0.4614378349807450 0.3388839801101600 T T T  
0.6690919997630900 0.8170932275262288 0.4621108699766978 F F F  
0.4563443067348629 0.1856957460417874 0.5415381954083784 F F F  
0.9563715435325619 0.3157762323396867 0.5415514049333012 F F F  
0.1684768759925106 0.6845410757490313 0.4614047933963619 F F F  
0.5163401794135183 0.6840621747006708 0.5172222351935218 F F F  
0.6122121268392959 0.3153938228045661 0.4863254931615089 F F F  
0.1121104352761861 0.1862923125396918 0.4862169103188876 F F F  
0.0164653504910319 0.8169379209085434 0.5170864510602016 F F F  
0.7737086930159478 0.4642121896258828 0.5098542901532497 F F F  
0.3547568199701061 0.5398845750144545 0.4913055491984935 F F F  
0.8548352112812623 0.9612879754852131 0.4913474116743402 F F F  
0.2736558171006749 0.0367285287095171 0.5095842622449496 F F F  
0.4364578605973435 0.0348585244096000 0.4598389770138454 F F F  
0.6931547229194095 0.9653791778681509 0.5438751113830449 F F F  
0.1930960752500894 0.5368671613790212 0.5435284188581946 F F F  
0.9363025789852344 0.4660265976351923 0.4598071447971463 F F F  
0.3745464228361111 0.8189143086570053 0.5811172624135954 T T T  
0.1567790712433682 0.1877480948294059 0.6615248569418004 T T T  
0.6551135645457231 0.3446508817642374 0.6582036833635491 T T T  
0.8746304806384877 0.6840106320399043 0.5815182608935511 T T T  
0.2239815934396471 0.6856061748830222 0.6407265429012897 T T T  
0.3206671701018216 0.3137684212787413 0.6093749237174582 T T T  
0.8180481948008402 0.1837763948823407 0.6071910993619601 T T T  
0.7181540946434912 0.8250794772394160 0.6409353983959705 T T T  
0.4860095420896841 0.4707650814275597 0.6282857397166535 T T T  
0.0619134030520969 0.5362848914812747 0.6100827177896642 T T T  
0.5630148264896453 0.9566162856608983 0.6112447302711411 T T T  
0.9789729108246312 0.0343288221507333 0.6338632826691445 T T T



0.1446451762836604 0.0341650751266066 0.5797569630898526 T T T  
0.4086389183537888 0.9511920727235973 0.6644997507904770 T T T  
0.9029603751994596 0.5440838992889261 0.6641581451685158 T T T  
0.6452498920220706 0.4780976019748238 0.5801230162068440 T T T  
0.0690650862805381 0.6816709473097406 0.6987623041977400 T T T  
0.3662390151156318 0.4344033148696392 0.7018876029518634 T T T  
0.8502163914645445 0.0663546629003841 0.7014312795499434 T T T  
0.5597541638417008 0.7432090065217917 0.6955101913270061 T T T  
0.2757725691813617 0.9240662761985430 0.3005315575980420 T T T  
0.5601971598534538 0.1855215352819501 0.3037926122734547 T T T  
0.7760044780974442 0.5802636858231073 0.3002824442257690 T T T  
0.0349573493836311 0.3125049379203773 0.2991660349352706 T T T  
0.0027468496066831 0.6247323558872885 0.6918664847805128 T T T  
0.3702010891543198 0.2477988745282645 0.6929391986466921 T T T  
0.8681765252629526 0.2470885306804539 0.6933352395633124 T T T  
0.6042351283455363 0.8694105306941216 0.7100401334147969 T T T  
0.1061411356715620 0.5208375057120392 0.6969984833161378 T T T  
0.4286431641405441 0.4757099300795947 0.7136724722844975 T T T  
0.7872895820885975 0.0770609024908183 0.7160111813695941 T T T  
0.5012531158224196 0.8484219560602139 0.6859980559023812 T T T  
0.2202671484355131 0.9667006409016048 0.2826924316249517 T T T  
0.2658176221472153 0.7396779966220534 0.3107549428992056 T T T  
0.5190560999881989 0.0323255712368170 0.3043699665294020 T T T  
0.6243877401261241 0.1170042770726745 0.3135519020835173 T T T  
0.7665539401399744 0.7633420202281659 0.3110585454183685 T T T  
0.7192435724857916 0.5410752170512405 0.2831073495675551 T T T  
0.0284808678394276 0.4945024440549495 0.3094138556472908 T T T  
0.9750877586509817 0.2762954793952957 0.2843563840277237 T T T  
0.6579447453730330 0.2375544594409266 0.7044666334646018 T T T

0.6520484754632787	0.2070164467186387	0.7593238018987192	T	T	T
0.6044837351861259	0.6291574555303644	0.6353379953611622	T	T	T
0.6487817750305567	0.6455289705310605	0.5195024736345744	F	F	F
0.6808022306140740	0.8678590557265413	0.3970877868100217	T	T	T

Ti O Ti O Ti O

1.0000000000000000		
14.2453041077000009	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.1680002212999998	0.0000000000000000
0.0000000000000000	0.0000000000000000	29.4789562224999990

Ti O H Co Ti

21 57 17 1 2

Selective dynamics

Direct

0.0215599168086614	0.1075513878870819	0.3670215528450409	T	T	T
0.1848815046208064	0.6330748289684363	0.3964600042183819	T	T	T
0.5180307888533244	0.3954974679762894	0.3649177334873336	T	T	T
0.7698529961411590	0.3500923570136008	0.3653601234644592	T	T	T
0.9388416562306844	0.6331999743081010	0.3972664155960602	T	T	T
0.4385168068258079	0.8666114663432162	0.3981809385340843	T	T	T
0.2704315693681208	0.1572608988967073	0.3634570894292779	T	T	T
0.7342005810289152	0.1367530326270341	0.4848529224897646	F	F	F
0.3956158154875027	0.8683481241609385	0.5172283169192724	F	F	F
0.8953822014665107	0.6325289816178099	0.5172296942882255	F	F	F
0.2344372928950307	0.3634625181788707	0.4844606095791164	F	F	F
0.4815241771643173	0.3615968561732217	0.4834047030315531	F	F	F
0.1487325421792534	0.8563983739423122	0.5193773182996253	F	F	F
0.9814354254124780	0.1396032612863678	0.4834948480823442	F	F	F

0.4437342659794313	0.1402754783867488	0.6061280453958325	T	T	T
0.1077098507918726	0.8951261521145766	0.6381844309699840	T	T	T
0.9439488538841230	0.3692567849539460	0.6064531475725853	T	T	T
0.1875641953276453	0.3667069624857295	0.6053084200633903	T	T	T
0.3575353060157233	0.6609659055611538	0.6377974218120513	T	T	T
0.8556599186783005	0.8450662067305142	0.6392849136711917	T	T	T
0.6880182526486062	0.1420378696225958	0.6030224084987720	T	T	T
0.6827157601402480	0.0751122785276032	0.7354216293988320	T	T	T
0.9712668626528378	0.8149368086759280	0.3412807238264742	T	T	T
0.7503335588125067	0.1865122563159473	0.4212635303860546	T	T	T
0.2508472685442520	0.3136710584274814	0.4209146868418622	T	T	T
0.4686761923297194	0.6881779189097340	0.3414086428043501	T	T	T
0.8086203550302901	0.6898310344122418	0.3950227445097347	T	T	T
0.9024909879197753	0.3130122987233522	0.3640057384458077	T	T	T
0.4046217155115676	0.1825357127931369	0.3619127533709863	T	T	T
0.3086154778054946	0.8166128370595157	0.3964045800698040	T	T	T
0.0667090887388082	0.4593713103105382	0.3899751951026744	T	T	T
0.6465141402887539	0.5397792768408621	0.3688994043630178	T	T	T
0.1475656954868168	0.9646639356736404	0.3686894242549764	T	T	T
0.5660329043177650	0.0393741800114929	0.3926862949713776	T	T	T
0.7226453445678466	0.0499809046854708	0.3378711109266918	T	T	T
0.9851917873131365	0.9634798813437487	0.4235153416157175	T	T	T
0.4846013328684067	0.5346411026093412	0.4232569759864764	T	T	T
0.2289791254882846	0.4616539161144241	0.3389191225000048	T	T	T
0.6690919997630900	0.8170932275262288	0.4621108699766978	F	F	F
0.4563443067348629	0.1856957460417874	0.5415381954083784	F	F	F
0.9563715435325619	0.3157762323396867	0.5415514049333012	F	F	F
0.1684768759925106	0.6845410757490313	0.4614047933963619	F	F	F
0.5163401794135183	0.6840621747006708	0.5172222351935218	F	F	F

0.6122121268392959	0.3153938228045661	0.4863254931615089	F	F	F
0.1121104352761861	0.1862923125396918	0.4862169103188876	F	F	F
0.0164653504910319	0.8169379209085434	0.5170864510602016	F	F	F
0.7737086930159478	0.4642121896258828	0.5098542901532497	F	F	F
0.3547568199701061	0.5398845750144545	0.4913055491984935	F	F	F
0.8548352112812623	0.9612879754852131	0.4913474116743402	F	F	F
0.2736558171006749	0.0367285287095171	0.5095842622449496	F	F	F
0.4364578605973435	0.0348585244096000	0.4598389770138454	F	F	F
0.6931547229194095	0.9653791778681509	0.5438751113830449	F	F	F
0.1930960752500894	0.5368671613790212	0.5435284188581946	F	F	F
0.9363025789852344	0.4660265976351923	0.4598071447971463	F	F	F
0.3748602651521520	0.8204264005318752	0.5812126130425229	T	T	T
0.1575176190710751	0.1890876433415425	0.6615316860159011	T	T	T
0.6539794162046867	0.3407267116448492	0.6587070136042096	T	T	T
0.8753961399510742	0.6847918473356063	0.5815788843300377	T	T	T
0.2245702173882823	0.6864050716148110	0.6411868412554534	T	T	T
0.3212518117079874	0.3187771427895865	0.6091654526879832	T	T	T
0.8176257178742942	0.1847596318289179	0.6078336040144648	T	T	T
0.7181832869779708	0.8187514803304750	0.6394697430073377	T	T	T
0.4868780218377793	0.4754957702664387	0.6264401596999888	T	T	T
0.0624681615785849	0.5365123265342571	0.6101385678271525	T	T	T
0.5635684324947787	0.9608748355758635	0.6119656498839188	T	T	T
0.9794519534180873	0.0337270124062134	0.6336423548342486	T	T	T
0.1453767419999436	0.0346525709028841	0.5798561928774941	T	T	T
0.4072329777267893	0.9600189793763229	0.6638387086312416	T	T	T
0.9040507095120397	0.5431251813287103	0.6640304527371497	T	T	T
0.6456273823590730	0.4790209390031049	0.5801899700191706	T	T	T
0.0700609532906695	0.6853835463274121	0.6990222604581894	T	T	T
0.3757034267475232	0.4466762665510589	0.7016690729550539	T	T	T

0.8488818757899474	0.0500708181867276	0.7011636893789165	T	T	T
0.5658812205641121	0.7267274628854175	0.6930147841340134	T	T	T
0.2761585877628800	0.9247801601542026	0.3005789855086542	T	T	T
0.5605243925437262	0.1870862899729271	0.3037911582633414	T	T	T
0.7768975274378034	0.5808953642077318	0.3004449218362300	T	T	T
0.0353960226639597	0.3123733146030581	0.2993308653834768	T	T	T
0.0038634827901184	0.6268782305937755	0.6928329100281950	T	T	T
0.3783584269792927	0.2583775346063819	0.6939413204689698	T	T	T
0.8670642228621472	0.2320953074987520	0.6955633132080294	T	T	T
0.6470070370048501	0.9204391134540305	0.7253590662825270	T	T	T
0.1074255789178413	0.5249979526500486	0.6980940884549310	T	T	T
0.4393970709328437	0.4913364843715347	0.7118363439418477	T	T	T
0.7838605664952760	0.0524987040145085	0.7169067131233549	T	T	T
0.5147235857710929	0.8542313894026980	0.6860047590670795	T	T	T
0.2214566776376729	0.9680656503858006	0.2822209703939784	T	T	T
0.2659378415516104	0.7403355919583843	0.3106165272520450	T	T	T
0.5193364701507853	0.0340637576583946	0.3039412293506183	T	T	T
0.6246421972775588	0.1180409210302139	0.3134800392191294	T	T	T
0.7670017068804791	0.7639704623211889	0.3110735028645078	T	T	T
0.7211629315730972	0.5416114369309299	0.2825148102587310	T	T	T
0.0282118882836284	0.4945661647476204	0.3093804192367041	T	T	T
0.9763896802553240	0.2748652689701604	0.2838298323220251	T	T	T
0.6618473003608719	0.2090759915531659	0.7134481874213208	T	T	T
0.6049485296434922	0.6293175501783137	0.6366626190038005	T	T	T
0.6487817750305567	0.6455289705310605	0.5195024736345744	F	F	F
0.6810184330361023	0.8682577525793401	0.3970060445989097	T	T	T

Ti O H Co

1.0000000000000000

14.2453041077000009 0.0000000000000000 0.0000000000000000  
0.0000000000000000 5.1680002212999998 0.0000000000000000  
0.0000000000000000 0.0000000000000000 29.4789562224999990

Ti O H Co Ti

21 57 17 1 2

Selective dynamics

Direct

0.0212767019130183 0.1070871431752154 0.3669751378943574 T T T  
0.1846133146723941 0.6329486355716698 0.3964698816805103 T T T  
0.5178935435482422 0.3951716342807508 0.3649767326236478 T T T  
0.7696798335080052 0.3498089597849535 0.3653866199439454 T T T  
0.9386668335740235 0.6328290566243322 0.3973506197753980 T T T  
0.4383033963312117 0.8663923932883720 0.3981030351909449 T T T  
0.2702463983217218 0.1571877669379638 0.3634718672816693 T T T  
0.7342005810289152 0.1367530326270341 0.4848529224897646 F F F  
0.3956158154875027 0.8683481241609385 0.5172283169192724 F F F  
0.8953822014665107 0.6325289816178099 0.5172296942882255 F F F  
0.2344372928950307 0.3634625181788707 0.4844606095791164 F F F  
0.4815241771643173 0.3615968561732217 0.4834047030315531 F F F  
0.1487325421792534 0.8563983739423122 0.5193773182996253 F F F  
0.9814354254124780 0.1396032612863678 0.4834948480823442 F F F  
0.4504240294137472 0.1441600285669999 0.6059683772542713 T T T  
0.1050334862107363 0.8977717475295603 0.6379621460019456 T T T  
0.9418892459311240 0.3738518995088044 0.6064175297902170 T T T  
0.1842567771544377 0.3680513971987519 0.6053484965446184 T T T  
0.3547098632293108 0.6407393441444467 0.6348280374827835 T T T  
0.8512750500590328 0.8534123607099162 0.6380063903031252 T T T  
0.6873031280356029 0.1462293307141693 0.6013962682823010 T T T  
0.6085566455867606 0.9344853217635344 0.7195713429278667 T T T

0.9710173125123709	0.8147254190483647	0.3412375763506998	T	T	T
0.7502039881676161	0.1863987131120185	0.4212658362432068	T	T	T
0.2507224016377489	0.3136135938848994	0.4209087066580244	T	T	T
0.4684607171282671	0.6877501427430561	0.3414074907383443	T	T	T
0.8084692267097168	0.6896553505321025	0.3950015433380912	T	T	T
0.9022955726181551	0.3130212201825718	0.3639792956659442	T	T	T
0.4044587102754794	0.1822333328833753	0.3618472874185122	T	T	T
0.3084095332569479	0.8166254304856585	0.3964310505515046	T	T	T
0.0665537094238642	0.4593127421673686	0.3899364607328695	T	T	T
0.6463237228503537	0.5395911492759259	0.3689074154990900	T	T	T
0.1473581522708216	0.9644904138181140	0.3686428909366369	T	T	T
0.5658650366946252	0.0392472397698235	0.3926720703295574	T	T	T
0.7224416830690130	0.0498040907442136	0.3378651551556773	T	T	T
0.9850610752118352	0.9633882782049328	0.4234905199658011	T	T	T
0.4843875170049635	0.5344748029412769	0.4232349017386693	T	T	T
0.2288548445755875	0.4616312670703880	0.3389077809937678	T	T	T
0.6690919997630900	0.8170932275262288	0.4621108699766978	F	F	F
0.4563443067348629	0.1856957460417874	0.5415381954083784	F	F	F
0.9563715435325619	0.3157762323396867	0.5415514049333012	F	F	F
0.1684768759925106	0.6845410757490313	0.4614047933963619	F	F	F
0.5163401794135183	0.6840621747006708	0.5172222351935218	F	F	F
0.6122121268392959	0.3153938228045661	0.4863254931615089	F	F	F
0.1121104352761861	0.1862923125396918	0.4862169103188876	F	F	F
0.0164653504910319	0.8169379209085434	0.5170864510602016	F	F	F
0.7737086930159478	0.4642121896258828	0.5098542901532497	F	F	F
0.3547568199701061	0.5398845750144545	0.4913055491984935	F	F	F
0.8548352112812623	0.9612879754852131	0.4913474116743402	F	F	F
0.2736558171006749	0.0367285287095171	0.5095842622449496	F	F	F
0.4364578605973435	0.0348585244096000	0.4598389770138454	F	F	F

0.6931547229194095 0.9653791778681509 0.5438751113830449 F F F  
0.1930960752500894 0.5368671613790212 0.5435284188581946 F F F  
0.9363025789852344 0.4660265976351923 0.4598071447971463 F F F  
0.3747438267873630 0.8208862972633143 0.5814697939389206 T T T  
0.1563664993639589 0.1904835644264538 0.6614696207848779 T T T  
0.6631400409028593 0.3343183435308756 0.6623535703933917 T T T  
0.8750183345371458 0.6892140514402000 0.5812221316284722 T T T  
0.2235902013383101 0.6892465258054087 0.6401298680862645 T T T  
0.3201308025394125 0.3117468261420013 0.6097996676653831 T T T  
0.8178265011243658 0.1902776913278536 0.6053659784315935 T T T  
0.7199244240337558 0.8235401216558689 0.6401999236958476 T T T  
0.4855614639843625 0.4676630113275055 0.6304467672831633 T T T  
0.0618083478562853 0.5413381439010460 0.6097342329617582 T T T  
0.5629180388623848 0.9604212751768170 0.6120957113688580 T T T  
0.9783801053198495 0.0443968538856915 0.6352394166958413 T T T  
0.1432251072448697 0.0368654748040896 0.5796794445675629 T T T  
0.4091137009926264 0.9534901810165868 0.6662228253906217 T T T  
0.9047944398019370 0.5569768777849408 0.6640187487771527 T T T  
0.6455304833911912 0.4751148410154886 0.5799592275722217 T T T  
0.0687774522918121 0.6870160530580154 0.6986965385644522 T T T  
0.3617958331309555 0.4436134363519703 0.7023948972899934 T T T  
0.8288939955196817 0.1103153402025062 0.6980111151538927 T T T  
0.5594726935765341 0.7284379728161877 0.6952293996315275 T T T  
0.2758089500452165 0.9243584611246820 0.3005574964880456 T T T  
0.5603738361568815 0.1869932549358879 0.3037501738211004 T T T  
0.7763540574354605 0.5804008350635249 0.3003867095480799 T T T  
0.0350751456552996 0.3128347005422496 0.2992437924846075 T T T  
0.0028230842008350 0.6273546474786156 0.6908986040084023 T T T  
0.3683802621566357 0.2561951287273976 0.6949578851983957 T T T



0.8722298122995422	0.2599451239905977	0.6943765157645962	T	T	T
0.1069887999955837	0.5281574210560485	0.6978093917488831	T	T	T
0.4218005312784325	0.4923934268156834	0.7161137296534931	T	T	T
0.7681355897107220	0.1945314715650966	0.6900432799542279	T	T	T
0.4694566865563076	0.8851983032744786	0.6809699015941775	T	T	T
0.2207524028685329	0.9674512368352381	0.2824316784475704	T	T	T
0.2656123425054969	0.7400170449500117	0.3106956067164831	T	T	T
0.5190656777236864	0.0342213646914599	0.3039479744139801	T	T	T
0.6244241860075399	0.1176743977037413	0.3135035683829076	T	T	T
0.7667823829853444	0.7635278306218993	0.3110844031813180	T	T	T
0.7200456075348206	0.5411885318427397	0.2828669490058324	T	T	T
0.0281428273366311	0.4949104868576804	0.3094006875171558	T	T	T
0.9757375385170209	0.2759029794397925	0.2840049192260659	T	T	T
0.6207712001461402	0.2338285217131240	0.6820870358071851	T	T	T
0.6697385193707606	0.8537177500727490	0.7253746140256158	T	T	T
0.6053671571643506	0.6382499288080694	0.6371661935720631	T	T	T
0.6487817750305567	0.6455289705310605	0.5195024736345744	F	F	F
0.6808689202112058	0.8680311834167033	0.3970530651441028	T	T	T

Ti O H Co

1.0000000000000000

14.2453041077000009 0.0000000000000000 0.0000000000000000

0.0000000000000000 5.1680002212999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 29.4789562224999990

Ti O H Co Ti

21 57 16 1 2

Selective dynamics

Direct

0.0213982198917167	0.1069616218356229	0.3669608192293311	T	T	T
--------------------	--------------------	--------------------	---	---	---

0.1847163697421883 0.6328909460820888 0.3964880281869435 T T T  
0.5181213307777870 0.3946522802291830 0.3650319857614759 T T T  
0.7698616898518620 0.3495945001717445 0.3653632154703589 T T T  
0.9387951111641779 0.6327781405477197 0.3974028109703516 T T T  
0.4384440127515296 0.8659980480878202 0.3980138127814798 T T T  
0.2703484004345947 0.1570220663356066 0.3634745208970940 T T T  
0.7342005810289152 0.1367530326270341 0.4848529224897646 F F F  
0.3956158154875027 0.8683481241609385 0.5172283169192724 F F F  
0.8953822014665107 0.6325289816178099 0.5172296942882255 F F F  
0.2344372928950307 0.3634625181788707 0.4844606095791164 F F F  
0.4815241771643173 0.3615968561732217 0.4834047030315531 F F F  
0.1487325421792534 0.8563983739423122 0.5193773182996253 F F F  
0.9814354254124780 0.1396032612863678 0.4834948480823442 F F F  
0.4509187766107948 0.1460290621627835 0.6057633136134360 T T T  
0.1056382739295415 0.8974979383110112 0.6379310019479615 T T T  
0.9423641279777420 0.3727264097182685 0.6062798134421232 T T T  
0.1845378122118276 0.3687021110889422 0.6052176582060045 T T T  
0.3553886627440415 0.6422520795663045 0.6350706113225747 T T T  
0.8522241069855967 0.8513578533009034 0.6384079167014706 T T T  
0.6882483312474383 0.1464855845318773 0.6015746232149972 T T T  
0.5605926073239184 0.9540696286292540 0.7112017340198802 T T T  
0.9711905768339456 0.8145353595110585 0.3412476308458385 T T T  
0.7503271951153421 0.1862911665010278 0.4212486983203691 T T T  
0.2508712106884500 0.3136431622645074 0.4209308086356848 T T T  
0.4686294252665683 0.6873629657714032 0.3414383536885818 T T T  
0.8085961849901163 0.6895168221594712 0.3950045666674272 T T T  
0.9024566845466419 0.3128385233256440 0.3639879743826645 T T T  
0.4046144478318349 0.1821174481451096 0.3618805380887752 T T T  
0.3085657345337674 0.8163916846312540 0.3964343128708462 T T T

0.0666644246887446	0.4592212279623433	0.3899628668210236	T	T	T
0.6464468795070926	0.5393887165474440	0.3689581191281856	T	T	T
0.1475696514248221	0.9644498847053929	0.3686545362105763	T	T	T
0.5659539151546612	0.0390205163872259	0.3926669829281234	T	T	T
0.7225981065069094	0.0496240788758115	0.3378492148432370	T	T	T
0.9851663202028097	0.9633361784969103	0.4234951155435208	T	T	T
0.4844650615486608	0.5342930817852043	0.4232783831707199	T	T	T
0.2290249621924199	0.4614191654359283	0.3389273215430613	T	T	T
0.6690919997630900	0.8170932275262288	0.4621108699766978	F	F	F
0.4563443067348629	0.1856957460417874	0.5415381954083784	F	F	F
0.9563715435325619	0.3157762323396867	0.5415514049333012	F	F	F
0.1684768759925106	0.6845410757490313	0.4614047933963619	F	F	F
0.5163401794135183	0.6840621747006708	0.5172222351935218	F	F	F
0.6122121268392959	0.3153938228045661	0.4863254931615089	F	F	F
0.1121104352761861	0.1862923125396918	0.4862169103188876	F	F	F
0.0164653504910319	0.8169379209085434	0.5170864510602016	F	F	F
0.7737086930159478	0.4642121896258828	0.5098542901532497	F	F	F
0.3547568199701061	0.5398845750144545	0.4913055491984935	F	F	F
0.8548352112812623	0.9612879754852131	0.4913474116743402	F	F	F
0.2736558171006749	0.0367285287095171	0.5095842622449496	F	F	F
0.4364578605973435	0.0348585244096000	0.4598389770138454	F	F	F
0.6931547229194095	0.9653791778681509	0.5438751113830449	F	F	F
0.1930960752500894	0.5368671613790212	0.5435284188581946	F	F	F
0.9363025789852344	0.4660265976351923	0.4598071447971463	F	F	F
0.3757248327167427	0.8242336795771312	0.5818768291708917	T	T	T
0.1575665731874049	0.1899338036914825	0.6613387604529672	T	T	T
0.6609086177978815	0.3252035587626828	0.6622858121555187	T	T	T
0.8757533034513475	0.6889594697767902	0.5812502967632244	T	T	T
0.2237008423922174	0.6891798960152761	0.6398635375878037	T	T	T

0.3208060863863651	0.3179188173049799	0.6087788593398468	T	T	T
0.8180920331550487	0.1898770588239329	0.6055166770967030	T	T	T
0.7206857002234850	0.8220669407169915	0.6395337028580538	T	T	T
0.4847416740661908	0.4682015401860238	0.6321541455729203	T	T	T
0.0620750805264552	0.5407195404202210	0.6097384628428462	T	T	T
0.5617994451421744	0.9580402777276910	0.6134178127430641	T	T	T
0.9789306837235898	0.0424390974945062	0.6348417790547891	T	T	T
0.1435651172872157	0.0369492117344786	0.5795524460329875	T	T	T
0.4019064704238158	0.9673586121045366	0.6662773981123121	T	T	T
0.9045218512611169	0.5526977847941243	0.6639553129605656	T	T	T
0.6442863036569467	0.4717926859555497	0.5796733318917983	T	T	T
0.0693835195907596	0.6869800654279976	0.6986993149045743	T	T	T
0.3530300177218846	0.4464454686377986	0.7024011976244763	T	T	T
0.8357748299910898	0.0996718304980075	0.6985299895425936	T	T	T
0.5815708762741436	0.7146524948577357	0.6980291862538412	T	T	T
0.2763403582261050	0.9240581322253193	0.3006107809277905	T	T	T
0.5605961267104352	0.1869749691789926	0.3037586730545366	T	T	T
0.7764902427962325	0.5802201499304018	0.3004265612133298	T	T	T
0.0353686582872455	0.3127876508762052	0.2993070999831699	T	T	T
0.0034073567467421	0.6269438323288116	0.6915403512260806	T	T	T
0.3553868482462693	0.2594740927693917	0.6938351502136448	T	T	T
0.8686633186242516	0.2665714232180478	0.6918724822453495	T	T	T
0.1075178161203481	0.5279854315241646	0.6979822317277702	T	T	T
0.4115825996798484	0.4789790443676856	0.7186081232922075	T	T	T
0.7693852647537939	0.1531611801619933	0.6979016225246835	T	T	T
0.4589560027949565	0.9616653321790442	0.6862762607463634	T	T	T
0.2216733874563059	0.9671137653100693	0.2822123978932191	T	T	T
0.2660335555856655	0.7396765941186723	0.3107236825625078	T	T	T
0.5192712181364536	0.0342467575204200	0.3038548722187289	T	T	T

0.6246474937378469	0.1174408609710414	0.3135079990079470	T	T	T
0.7667817128226770	0.7633526537531058	0.3110768496502300	T	T	T
0.7203879997182586	0.5409784857850894	0.2827567948219092	T	T	T
0.0282903471295075	0.4948093301554657	0.3094651467788331	T	T	T
0.9762546500793348	0.2757612916681704	0.2838791071983131	T	T	T
0.6145917330039165	0.2202881600665792	0.6795195492292091	T	T	T
0.6059698209446496	0.6370386533804341	0.6388965520318705	T	T	T
0.6487817750305567	0.6455289705310605	0.5195024736345744	F	F	F
0.6810551506195919	0.8678109569463023	0.3970851876280412	T	T	T

Ti O H Co

1.0000000000000000

14.2453041077000009 0.0000000000000000 0.0000000000000000

0.0000000000000000 5.1680002212999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 29.4789562224999990

Ti O H Co Ti

21 57 15 1 2

Selective dynamics

Direct

0.0213813194591551	0.1073908368951753	0.3669761468754779	T	T	T
0.1847129987475138	0.6329197999107864	0.3965054749083289	T	T	T
0.5176518780680970	0.3959592975073337	0.3648901218633005	T	T	T
0.7697209543031118	0.3501254955762854	0.3654571239863735	T	T	T
0.9387079710578187	0.6330864104248026	0.3972819461443204	T	T	T
0.4382689644217518	0.8670037166535876	0.3983277471753863	T	T	T
0.2701829549409121	0.1571375010007562	0.3634299575007640	T	T	T
0.7342005810289152	0.1367530326270341	0.4848529224897646	F	F	F
0.3956158154875027	0.8683481241609385	0.5172283169192724	F	F	F
0.8953822014665107	0.6325289816178099	0.5172296942882255	F	F	F

0.2344372928950307 0.3634625181788707 0.4844606095791164 F F F  
0.4815241771643173 0.3615968561732217 0.4834047030315531 F F F  
0.1487325421792534 0.8563983739423122 0.5193773182996253 F F F  
0.9814354254124780 0.1396032612863678 0.4834948480823442 F F F  
0.4392843856244487 0.1483647713360595 0.6066505564947694 T T T  
0.1084190506179770 0.8978232634692513 0.6380498053102414 T T T  
0.9445577682605504 0.3715650659367610 0.6063755439425789 T T T  
0.1866422651353031 0.3712373188999715 0.6051611622383343 T T T  
0.3593318273256391 0.6637076612210906 0.6381125393228128 T T T  
0.8540473064957941 0.8502047184375595 0.6379929016068945 T T T  
0.6896396844556829 0.1452890329004535 0.6013815525128310 T T T  
0.5860783736461320 0.9419262042183625 0.7149887781237255 T T T  
0.9708875301100374 0.8149482582849172 0.3412486178559217 T T T  
0.7502647146396729 0.1865205161050467 0.4213480900521098 T T T  
0.2505613557267752 0.3134029544846124 0.4208794092702099 T T T  
0.4685787568583926 0.6886044277531292 0.3413758613671060 T T T  
0.8084726193929809 0.6895420262739741 0.3950336823788406 T T T  
0.9022672607665591 0.3130277381688321 0.3639860778528008 T T T  
0.4043870765330625 0.1825472791471568 0.3619429878390005 T T T  
0.3084019664382710 0.8164612475732331 0.3964101324436790 T T T  
0.0664943210957818 0.4593280381137628 0.3899209920938529 T T T  
0.6463342019006365 0.5397048463011557 0.3688971940749849 T T T  
0.1473175267052195 0.9643781070145260 0.3685965330105239 T T T  
0.5659271034857717 0.0393442455603310 0.3927119312055096 T T T  
0.7224190326329276 0.0497507598454946 0.3379604789467384 T T T  
0.9850669264631803 0.9635502342472009 0.4234929993373174 T T T  
0.4844415049093396 0.5348766384091301 0.4232043356591356 T T T  
0.2288646230558618 0.4615217938398396 0.3388821850799274 T T T  
0.6690919997630900 0.8170932275262288 0.4621108699766978 F F F

0.4563443067348629 0.1856957460417874 0.5415381954083784 F F F  
0.9563715435325619 0.3157762323396867 0.5415514049333012 F F F  
0.1684768759925106 0.6845410757490313 0.4614047933963619 F F F  
0.5163401794135183 0.6840621747006708 0.5172222351935218 F F F  
0.6122121268392959 0.3153938228045661 0.4863254931615089 F F F  
0.1121104352761861 0.1862923125396918 0.4862169103188876 F F F  
0.0164653504910319 0.8169379209085434 0.5170864510602016 F F F  
0.7737086930159478 0.4642121896258828 0.5098542901532497 F F F  
0.3547568199701061 0.5398845750144545 0.4913055491984935 F F F  
0.8548352112812623 0.9612879754852131 0.4913474116743402 F F F  
0.2736558171006749 0.0367285287095171 0.5095842622449496 F F F  
0.4364578605973435 0.0348585244096000 0.4598389770138454 F F F  
0.6931547229194095 0.9653791778681509 0.5438751113830449 F F F  
0.1930960752500894 0.5368671613790212 0.5435284188581946 F F F  
0.9363025789852344 0.4660265976351923 0.4598071447971463 F F F  
0.3766539884450127 0.8161664727662074 0.5809388796070328 T T T  
0.1574655598314359 0.1918898386681067 0.6614922850899624 T T T  
0.6574001001368834 0.3431667893353822 0.6611439390447147 T T T  
0.8751793389956746 0.6887615172183655 0.5812821621466724 T T T  
0.2237414155171848 0.6874797014874531 0.6401722647972581 T T T  
0.3193942253182697 0.3182057134627566 0.6073232331302018 T T T  
0.8178566271581678 0.1918205826955879 0.6058375639524853 T T T  
0.7192358067410702 0.8310100053327338 0.6399434976067980 T T T  
0.4850072676497115 0.4702502138772404 0.6306431348145681 T T T  
0.0614523946905742 0.5413416657779895 0.6098546232630188 T T T  
0.5629062581169343 -0.0442875043997232 0.6131787926211281 T T T  
0.9783148953347641 0.0408091647360299 0.6347070973541428 T T T  
0.1436351419053876 0.0369248149022979 0.5796184257998463 T T T  
0.3999631866744334 0.9672223717767189 0.6632149344164008 T T T

0.9031347942323001	0.5511454322846081	0.6641293384513011	T	T	T
0.6452253964440626	0.4767572775694788	0.5798931045194651	T	T	T
0.0697028360575645	0.6867087121342044	0.6987824903094589	T	T	T
0.3572622372518444	0.4376565585826587	0.7018480081075181	T	T	T
0.8383484383388458	0.0937182820685205	0.6992266134152355	T	T	T
0.5695849172352606	0.7187161169032993	0.6977809047175946	T	T	T
0.2761693123231053	0.9239833125024562	0.3006014630580255	T	T	T
0.5600954092386483	0.1859590689515036	0.3038473574324775	T	T	T
0.7762231422328556	0.5798696477465033	0.3003696739423189	T	T	T
0.0348562138155313	0.3128525745887111	0.2992401301748744	T	T	T
0.0036060492819932	0.6285403135663411	0.6919645640486640	T	T	T
0.3655772098795285	0.2512356257244324	0.6931007298610444	T	T	T
0.8646912503632935	0.2681947598507847	0.6913752384795280	T	T	T
0.1072374241127881	0.5265668978788371	0.6976875981919257	T	T	T
0.4132346222790120	0.4825737191800145	0.7192285224717718	T	T	T
0.7708901085572328	0.1259802562354994	0.7022777563066347	T	T	T
0.2214416418098451	0.9668333732606256	0.2822331981220207	T	T	T
0.2659144054795857	0.7395924151142694	0.3107322971935488	T	T	T
0.5189510219035780	0.0327412261534078	0.3043238148024286	T	T	T
0.6242296468002030	0.1173460512510988	0.3135746915819753	T	T	T
0.7667829969968203	0.7630460914210667	0.3110202521327122	T	T	T
0.7197957001533322	0.5407152929137872	0.2829385162050486	T	T	T
0.0277778296964117	0.4948885351199803	0.3093815817679511	T	T	T
0.9755344689641630	0.2754144135243100	0.2840308417873229	T	T	T
0.6112743981668661	0.2417207651901262	0.6787207586326556	T	T	T
0.6034096012056285	0.6468031061538878	0.6354173078820734	T	T	T
0.6487817750305567	0.6455289705310605	0.5195024736345744	F	F	F
0.6807486544054474	0.8681826600974436	0.3969252678660846	T	T	T



Ti O H Co

1.0000000000000000

14.2453041077000009 0.0000000000000000 0.0000000000000000

0.0000000000000000 5.1680002212999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 29.4789562224999990

Ti O H Co Ti

21 55 15 1 2

Selective dynamics

Direct

0.0214503933789604 0.1074787218364907 0.3670054775065194 T T T

0.1847529608252368 0.6332304890425653 0.3965918978882200 T T T

0.5176060762374289 0.3962116072797441 0.3648881671323687 T T T

0.7698040738808525 0.3503670840602595 0.3655030799922851 T T T

0.9388001194073897 0.6332129056175124 0.3972429445177130 T T T

0.4382125546049604 0.8671720456885301 0.3983223214145749 T T T

0.2701610562298145 0.1576571859297912 0.3633754791819792 T T T

0.7342005810289152 0.1367530326270341 0.4848529224897646 F F F

0.3956158154875027 0.8683481241609385 0.5172283169192724 F F F

0.8953822014665107 0.6325289816178099 0.5172296942882255 F F F

0.2344372928950307 0.3634625181788707 0.4844606095791164 F F F

0.4815241771643173 0.3615968561732217 0.4834047030315531 F F F

0.1487325421792534 0.8563983739423122 0.5193773182996253 F F F

0.9814354254124780 0.1396032612863678 0.4834948480823442 F F F

0.4437936779415136 0.1426255521572428 0.6069185803302716 T T T

0.1092576203508894 0.8963481814787905 0.6377408135114357 T T T

0.9455925335353115 0.3718861260784609 0.6065541938516573 T T T

0.1893290480785449 0.3692916737837157 0.6052533592348092 T T T

0.3606113192733203 0.6609271529076614 0.6379512041915336 T T T

0.8549361745966019 0.8502311830529014 0.6381753121809376 T T T

0.6896158821308968	0.1333672879867243	0.6020892018898137	T	T	T
0.9709073547544403	0.8151653373677645	0.3412335652299974	T	T	T
0.7503040425634181	0.1866643493479674	0.4213866392770016	T	T	T
0.2506143382201261	0.3137741919915620	0.4208205569009665	T	T	T
0.4685297476993004	0.6887362474788359	0.3413519727645229	T	T	T
0.8084810326128185	0.6895575315777828	0.3950235316904126	T	T	T
0.9022942612922308	0.3132057398026031	0.3638990956592436	T	T	T
0.4044264583403858	0.1826100913703521	0.3618686529281291	T	T	T
0.3083836081865248	0.8166730313739730	0.3963773111765898	T	T	T
0.0664829496594084	0.4594452462485802	0.3899016091162489	T	T	T
0.6463512814280112	0.5399481783575524	0.3688893570862790	T	T	T
0.1473352790079465	0.9646327997467918	0.3686077452129889	T	T	T
0.5659312466261569	0.0394792110659619	0.3926872688761927	T	T	T
0.7224136067682069	0.0499207477042392	0.3379941816602865	T	T	T
0.9850340025162669	0.9635586247631031	0.4234703011308001	T	T	T
0.4844675523950998	0.5350319338404543	0.4231861333685332	T	T	T
0.2287860994932650	0.4618204962699310	0.3388269094452389	T	T	T
0.6690919997630900	0.8170932275262288	0.4621108699766978	F	F	F
0.4563443067348629	0.1856957460417874	0.5415381954083784	F	F	F
0.9563715435325619	0.3157762323396867	0.5415514049333012	F	F	F
0.1684768759925106	0.6845410757490313	0.4614047933963619	F	F	F
0.5163401794135183	0.6840621747006708	0.5172222351935218	F	F	F
0.6122121268392959	0.3153938228045661	0.4863254931615089	F	F	F
0.1121104352761861	0.1862923125396918	0.4862169103188876	F	F	F
0.0164653504910319	0.8169379209085434	0.5170864510602016	F	F	F
0.7737086930159478	0.4642121896258828	0.5098542901532497	F	F	F
0.3547568199701061	0.5398845750144545	0.4913055491984935	F	F	F
0.8548352112812623	0.9612879754852131	0.4913474116743402	F	F	F
0.2736558171006749	0.0367285287095171	0.5095842622449496	F	F	F

0.4364578605973435 0.0348585244096000 0.4598389770138454 F F F  
0.6931547229194095 0.9653791778681509 0.5438751113830449 F F F  
0.1930960752500894 0.5368671613790212 0.5435284188581946 F F F  
0.9363025789852344 0.4660265976351923 0.4598071447971463 F F F  
0.3775116446179798 0.8151001115020747 0.5811149176355577 T T T  
0.1577841102799560 0.1906946302134974 0.6613804899231183 T T T  
0.6542105586097997 0.3390494660925599 0.6624582191624667 T T T  
0.8749436492655199 0.6886996650449476 0.5814835422940577 T T T  
0.2244592128558964 0.6877504160027017 0.6397975460295723 T T T  
0.3204870885435041 0.3148070458757343 0.6079521877166492 T T T  
0.8172064904613520 0.1918122774141357 0.6064477660786948 T T T  
0.7187363864908224 0.8237420430498487 0.6403858136152658 T T T  
0.4864389368553159 0.4695695262301637 0.6322475977627114 T T T  
0.0616981565093735 0.5403954375189828 0.6098938318688040 T T T  
0.5621058656033174 0.9606084120605001 0.6132465145934269 T T T  
0.9782856897338393 0.0408779028803301 0.6350520620747735 T T T  
0.1437844490125178 0.0364481471719956 0.5794492795327246 T T T  
0.4024422703739509 0.9609180036615743 0.6642648066375278 T T T  
0.9044694448398463 0.5524708228446074 0.6644342863940711 T T T  
0.6454382812119941 0.4692178049087663 0.5797051294548692 T T T  
0.0711060142558887 0.6848902982138769 0.6987285448402332 T T T  
0.3513237630367129 0.4242601374419907 0.7011034620113559 T T T  
0.8328915031503368 0.1015400543495307 0.6987036467581066 T T T  
0.2757126060729420 0.9243374599587987 0.3005233870929340 T T T  
0.5603311235146050 0.1867923413406066 0.3037894145663327 T T T  
0.7759172280448373 0.5797071403028697 0.3003038530224704 T T T  
0.0351011099850966 0.3124277498958796 0.2991754263590972 T T T  
0.0049059379954113 0.6276030679823134 0.6918130100860707 T T T  
0.3629074184153422 0.2393257208203014 0.6917618736826115 T T T

0.8659990409385142	0.2681739129005757	0.6918541564473303	T	T	T
0.1084232613879952	0.5244031133740328	0.6970851607239558	T	T	T
0.4005561764555483	0.4673395089766837	0.7226777126543282	T	T	T
0.7665588778777005	0.1533286845721377	0.6966707584713089	T	T	T
0.2204914803695376	0.9672169727741909	0.2824982732370706	T	T	T
0.2656107973362808	0.7399601375645565	0.3107259992872992	T	T	T
0.5190730194757268	0.0338174223164607	0.3041661499470325	T	T	T
0.6243729528856223	0.1178232277343873	0.3135987731964799	T	T	T
0.7666619414389885	0.7628868545271582	0.3109795006966687	T	T	T
0.7190560507215931	0.5404774282110533	0.2831990133645257	T	T	T
0.0286895897890424	0.4945557486325229	0.3093602133195728	T	T	T
0.9753903758300959	0.2763797338331426	0.2842116966810385	T	T	T
0.5974345121621220	0.2486913612400085	0.6724887978756710	T	T	T
0.6058065413999046	0.6366496807667054	0.6315497895224136	T	T	T
0.6487817750305567	0.6455289705310605	0.5195024736345744	F	F	F
0.6807327761756677	0.8683623698656783	0.3968651878897071	T	T	T

Ti O H Co

1.000000000000000		
14.2453041077000009	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.1680002212999998	0.0000000000000000
0.0000000000000000	0.0000000000000000	29.4789562224999990

Ti O H Co Ti

21 55 14 1 2

Selective dynamics

Direct

0.0214724361085001	0.1076737174418542	0.3670725986045498	T	T	T
0.1847754978996346	0.6332115317874598	0.3965519349657027	T	T	T
0.5177364685075161	0.3959431278570795	0.3649064321787855	T	T	T

0.7697340788357334 0.3498944121601741 0.3653915995325664 T T T  
0.9387196864875923 0.6332985079139087 0.3971345935104980 T T T  
0.4382838622504735 0.8669189202474580 0.3982984689767737 T T T  
0.2702851682964154 0.1574716636629322 0.3634214692374221 T T T  
0.7342005810289152 0.1367530326270341 0.4848529224897646 F F F  
0.3956158154875027 0.8683481241609385 0.5172283169192724 F F F  
0.8953822014665107 0.6325289816178099 0.5172296942882255 F F F  
0.2344372928950307 0.3634625181788707 0.4844606095791164 F F F  
0.4815241771643173 0.3615968561732217 0.4834047030315531 F F F  
0.1487325421792534 0.8563983739423122 0.5193773182996253 F F F  
0.9814354254124780 0.1396032612863678 0.4834948480823442 F F F  
0.4443313462849851 0.1358112073699763 0.6067312085483031 T T T  
0.1095423488289688 0.8923613811891473 0.6380828546729778 T T T  
0.9451047933258951 0.3653530398346856 0.6066434030197582 T T T  
0.1891643765369587 0.3656783417198847 0.6051138697413798 T T T  
0.3601396973990576 0.6571453039595136 0.6378923182644313 T T T  
0.8560332038024165 0.8445187055965598 0.6379785113834008 T T T  
0.6881716946297448 0.1298173297639144 0.6048136877249678 T T T  
0.9709623620445808 0.8152946055944097 0.3412542519802415 T T T  
0.7503099340307327 0.1862268057666903 0.4212338078016644 T T T  
0.2506684762004286 0.3136276092603401 0.4208718178651503 T T T  
0.4684240632212343 0.6883265635238414 0.3413855988602226 T T T  
0.8084487688869425 0.6894080306439422 0.3950055338896982 T T T  
0.9023936618836561 0.3132649676582067 0.3638296666896931 T T T  
0.4044500654459480 0.1824168340196775 0.3618716580448871 T T T  
0.3083864228046708 0.8166621606343860 0.3964395439351089 T T T  
0.0665184890834951 0.4593613211333654 0.3899216445446782 T T T  
0.6463778967442316 0.5396862120688127 0.3688418676315917 T T T  
0.1473704862966567 0.9646113436072745 0.3686624865326535 T T T

0.5658888624722519 0.0393383996455039 0.3926630721983283 T T T  
0.7223931916626505 0.0497124627136402 0.3378573971493156 T T T  
0.9850659317411470 0.9634911510353228 0.4235049627339516 T T T  
0.4844704771774281 0.5348320851217008 0.4232028112296986 T T T  
0.2288512371714580 0.4617995662873237 0.3388878793047931 T T T  
0.6690919997630900 0.8170932275262288 0.4621108699766978 F F F  
0.4563443067348629 0.1856957460417874 0.5415381954083784 F F F  
0.9563715435325619 0.3157762323396867 0.5415514049333012 F F F  
0.1684768759925106 0.6845410757490313 0.4614047933963619 F F F  
0.5163401794135183 0.6840621747006708 0.5172222351935218 F F F  
0.6122121268392959 0.3153938228045661 0.4863254931615089 F F F  
0.1121104352761861 0.1862923125396918 0.4862169103188876 F F F  
0.0164653504910319 0.8169379209085434 0.5170864510602016 F F F  
0.7737086930159478 0.4642121896258828 0.5098542901532497 F F F  
0.3547568199701061 0.5398845750144545 0.4913055491984935 F F F  
0.8548352112812623 0.9612879754852131 0.4913474116743402 F F F  
0.2736558171006749 0.0367285287095171 0.5095842622449496 F F F  
0.4364578605973435 0.0348585244096000 0.4598389770138454 F F F  
0.6931547229194095 0.9653791778681509 0.5438751113830449 F F F  
0.1930960752500894 0.5368671613790212 0.5435284188581946 F F F  
0.9363025789852344 0.4660265976351923 0.4598071447971463 F F F  
0.3771879643618721 0.8139967492242584 0.5810526690184316 T T T  
0.1583726667723586 0.1868749676094332 0.6614526705776349 T T T  
0.6559863420212106 0.3462393851731408 0.6577448857374580 T T T  
0.8749341951315946 0.6827559404009464 0.5816792830604722 T T T  
0.2248713704718978 0.6839000301436514 0.6401099453899289 T T T  
0.3212868445062539 0.3127474879703278 0.6080319542739259 T T T  
0.8183747938961600 0.1814667421655866 0.6067862503927209 T T T  
0.7187014441408858 0.8160538525841018 0.6409151068775298 T T T

0.4873014119630693 0.4687569172917228 0.6301094293496025 T T T  
0.0620359638609759 0.5346876059153051 0.6101183660714298 T T T  
0.5626548985072507 0.9492782335882481 0.6127823460845118 T T T  
0.9790571190778435 0.0339286169681368 0.6352285558322252 T T T  
0.1441391116202162 0.0334696675787509 0.5796923798831001 T T T  
0.4028844383310787 0.9570441505942897 0.6638220271441175 T T T  
0.9042575996093309 0.5443325162689187 0.6644644070715334 T T T  
0.6444840465576733 0.4655727925801075 0.5793934250970620 T T T  
0.0712560300247281 0.6796158154490052 0.6988278496874829 T T T  
0.3573259708662815 0.4220510663991042 0.7007902023005300 T T T  
0.8362353965601088 0.0891684672946132 0.6996641261077632 T T T  
0.2756288496692049 0.9244975437916546 0.3005456123439194 T T T  
0.5602230456578607 0.1869918906162752 0.3037350459134028 T T T  
0.7762415777585224 0.5804108223206785 0.3003578517204186 T T T  
0.0356509118216282 0.3118789535892197 0.2991471959237506 T T T  
0.0051569502967586 0.6213894432672641 0.6919739368382569 T T T  
0.3670939563783372 0.2363356717315883 0.6914058720095219 T T T  
0.8634429597913678 0.2626009501817722 0.6917018366692728 T T T  
0.1087313177132780 0.5193765045419103 0.6972547462657146 T T T  
0.4100163594918381 0.4636909835934317 0.7205025724242734 T T T  
0.7687643679713958 0.1231359833925216 0.7017633766892407 T T T  
0.2203546793900187 0.9674065321404849 0.2825636525501233 T T T  
0.2655676760008424 0.7400654503770546 0.3107192298040268 T T T  
0.5188766310222502 0.0342553947249628 0.3040079651048517 T T T  
0.6242664149170515 0.1176943746054182 0.3135066292462313 T T T  
0.7665943978327772 0.7634065288843248 0.3110843039522756 T T T  
0.7198377303472129 0.5409830513190194 0.2829329281229622 T T T  
0.0294819227781121 0.4940829245380457 0.3092672926643949 T T T  
0.9759571278889866 0.2763655168874420 0.2841370634098773 T T T

0.6068357347631118	0.6194022438876633	0.6319138709465639	T	T	T
0.6487817750305567	0.6455289705310605	0.5195024736345744	F	F	F
0.6807646344060192	0.8681946665655722	0.3969407319227403	T	T	T

Ti O Ti O Ti O

1.0000000000000000

14.2453041077000009 0.0000000000000000 0.0000000000000000

0.0000000000000000 5.1680002212999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 29.4789562224999990

Ti O H Co Ti

21 56 16 1 2

Selective dynamics

Direct

0.0213857415974584	0.1072491500621199	0.3670790613301138	T	T	T
0.1846750075748692	0.6330151544844386	0.3964811960437442	T	T	T
0.5179419860550855	0.3954410676023908	0.3649175945626758	T	T	T
0.7696297813024251	0.3493397640645880	0.3652975242111105	T	T	T
0.9385681268421070	0.6329607430340062	0.3972229383672358	T	T	T
0.4383710427066121	0.8665294537535482	0.3981959530643195	T	T	T
0.2703362387201804	0.1572275602224801	0.3634776472453933	T	T	T
0.7342005810289152	0.1367530326270341	0.4848529224897646	F	F	F
0.3956158154875027	0.8683481241609385	0.5172283169192724	F	F	F
0.8953822014665107	0.6325289816178099	0.5172296942882255	F	F	F
0.2344372928950307	0.3634625181788707	0.4844606095791164	F	F	F
0.4815241771643173	0.3615968561732217	0.4834047030315531	F	F	F
0.1487325421792534	0.8563983739423122	0.5193773182996253	F	F	F
0.9814354254124780	0.1396032612863678	0.4834948480823442	F	F	F
0.4469575508970534	0.1371532702691814	0.6060422645295068	T	T	T
0.1046930207343585	0.8930721243765418	0.6349663864669440	T	T	T



0.9412372457302750	0.3668931949921824	0.6068515880850541	T	T	T
0.1890378547443402	0.3682451552133479	0.6065114434843313	T	T	T
0.3592109255188354	0.6540720194746750	0.6365893032359866	T	T	T
0.8521827223822847	0.8393377347418974	0.6381501110209704	T	T	T
0.6864465004622647	0.1415716521338724	0.6041137256527929	T	T	T
0.9709828591365054	0.8150342333761117	0.3412482563614031	T	T	T
0.7502713574735294	0.1859213170961587	0.4211168616571160	T	T	T
0.2507054907448285	0.3136233072763942	0.4208871324777627	T	T	T
0.4684952944511531	0.6879301980353741	0.3413732853830708	T	T	T
0.8084558537709142	0.6894681519178966	0.3949760232748027	T	T	T
0.9023957222468835	0.3131204698405143	0.3638646654453291	T	T	T
0.4044930631805944	0.1821906098543898	0.3618367670967716	T	T	T
0.3084512576136796	0.8166177111286259	0.3964167607558649	T	T	T
0.0665699165190697	0.4592908931474436	0.3899189291929724	T	T	T
0.6463719332370358	0.5394874897288228	0.3688042630184608	T	T	T
0.1474238245678578	0.9644744178109295	0.3686192280362733	T	T	T
0.5658729088384400	0.0391870201902274	0.3926446191934968	T	T	T
0.7224913678176894	0.0496682965568687	0.3377143022643744	T	T	T
0.9850952240767715	0.9632648867823712	0.4235232718872593	T	T	T
0.4844429014828033	0.5344888142781622	0.4232012747775717	T	T	T
0.2288513867503356	0.4615655290367490	0.3388929446512826	T	T	T
0.6690919997630900	0.8170932275262288	0.4621108699766978	F	F	F
0.4563443067348629	0.1856957460417874	0.5415381954083784	F	F	F
0.9563715435325619	0.3157762323396867	0.5415514049333012	F	F	F
0.1684768759925106	0.6845410757490313	0.4614047933963619	F	F	F
0.5163401794135183	0.6840621747006708	0.5172222351935218	F	F	F
0.6122121268392959	0.3153938228045661	0.4863254931615089	F	F	F
0.1121104352761861	0.1862923125396918	0.4862169103188876	F	F	F
0.0164653504910319	0.8169379209085434	0.5170864510602016	F	F	F

0.7737086930159478 0.4642121896258828 0.5098542901532497 F F F  
0.3547568199701061 0.5398845750144545 0.4913055491984935 F F F  
0.8548352112812623 0.9612879754852131 0.4913474116743402 F F F  
0.2736558171006749 0.0367285287095171 0.5095842622449496 F F F  
0.4364578605973435 0.0348585244096000 0.4598389770138454 F F F  
0.6931547229194095 0.9653791778681509 0.5438751113830449 F F F  
0.1930960752500894 0.5368671613790212 0.5435284188581946 F F F  
0.9363025789852344 0.4660265976351923 0.4598071447971463 F F F  
0.3754969040450236 0.8176812796600349 0.5810827851055153 T T T  
0.1552363579624802 0.1850618365805308 0.6615434758314761 T T T  
0.6529221407606671 0.3384859161938149 0.6586438334146946 T T T  
0.8751129669920767 0.6850332016489591 0.5812605406388018 T T T  
0.2260348341970583 0.6884328761340937 0.6392114491396237 T T T  
0.3207599778267918 0.3093561193512909 0.6099004222214239 T T T  
0.8174448973549630 0.1837595743184844 0.6080734061068882 T T T  
0.7179714078147935 0.8190133681500023 0.6403699517253226 T T T  
0.4855810881164190 0.4678136130283660 0.6290921456365557 T T T  
0.0611175222594685 0.5398628190772820 0.6127349957314093 T T T  
0.5627177388505307 0.9539028321376493 0.6106250493351926 T T T  
0.9790962646738769 0.0326208593216515 0.6330959170642090 T T T  
0.1446399180358074 0.0382913062709285 0.5791571720958916 T T T  
0.4099217282750847 0.9482810812868058 0.6650604479325061 T T T  
0.8976322165943535 0.5388265846972812 0.6635670184390959 T T T  
0.6443782304757129 0.4732288507467479 0.5798245385587997 T T T  
0.0908771092892355 0.6935340652824781 0.7033411716967634 T T T  
0.3625555920085771 0.4270568174713028 0.7023222004911981 T T T  
0.8511555930619358 0.0707304854709769 0.7019294286022110 T T T  
0.5669217824296339 0.7666289893121695 0.6946507744497630 T T T  
0.2755946144669726 0.9243212453251084 0.3005031530188392 T T T

0.5602170446937645	0.1859040996091093	0.3037452152084665	T	T	T
0.7762705088681940	0.5808892984795071	0.3002865442391820	T	T	T
0.0351034425497842	0.3122918519603245	0.2991443924185723	T	T	T
0.0960437492470860	0.5105504904794022	0.6936151778822189	T	T	T
0.3696984348458691	0.2422378756933330	0.6924138116163154	T	T	T
0.9075708894533854	0.0234985233595555	0.7187169716330742	T	T	T
0.6144254348126523	0.9016124782796491	0.6994199737211398	T	T	T
0.1514138885789226	0.7292701231834389	0.7175479491003736	T	T	T
0.4223067809899327	0.4687023664031018	0.7168140014331943	T	T	T
0.8615990741220260	0.2549769077292882	0.6919856714260120	T	T	T
0.5057095499889016	0.8617900409685038	0.6854684616714217	T	T	T
0.2198334795730294	0.9669650336355786	0.2828422000304285	T	T	T
0.2657421321705111	0.7398962632438257	0.3107486799883804	T	T	T
0.5190602894871402	0.0327904889572875	0.3042814095186751	T	T	T
0.6244194654407855	0.1173399736043424	0.3134864036180454	T	T	T
0.7667316966560845	0.7639026175378516	0.3110940349459082	T	T	T
0.7196068050929273	0.5418227935450829	0.2830300264825173	T	T	T
0.0289892230517178	0.4943203646740232	0.3094070552029725	T	T	T
0.9750282584788574	0.2768573548286206	0.2844719653443810	T	T	T
0.6055785166649402	0.6234242049032703	0.6350271267039491	T	T	T
0.6487817750305567	0.6455289705310605	0.5195024736345744	F	F	F
0.6808436189302811	0.8678647002148805	0.3971278423564272	T	T	T

=====Structures for Co not in a line=====

Ti O Ti O Ti O

1.0000000000000000

14.2453041077000009 0.0000000000000000 0.0000000000000000

0.0000000000000000 5.1680002212999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 29.4789562224999990

Ti O H Co

21 57 18 3

### Selective dynamics

#### Direct

0.0229269439658362	0.1066307661498534	0.3675895019873205	T	T	T
0.1855265275601233	0.6245830575756987	0.3964359074155691	T	T	T
0.5239877009071590	0.4019979482004275	0.3655288951125518	T	T	T
0.7676577929074611	0.3527907791616260	0.3657578290375430	T	T	T
0.9369473925479603	0.6342758642166617	0.3975643766829947	T	T	T
0.4409249910565388	0.8638196507029406	0.3997623394548631	T	T	T
0.2745850228651409	0.1521364336126760	0.3679610922627341	T	T	T
0.7342005810289152	0.1367530326270341	0.4848529224897646	F	F	F
0.3956158154875027	0.8683481241609385	0.5172283169192724	F	F	F
0.8953822014665107	0.6325289816178099	0.5172296942882255	F	F	F
0.6487817750305567	0.6455289705310605	0.5195024736345744	F	F	F
0.4815241771643173	0.3615968561732217	0.4834047030315531	F	F	F
0.1487325421792534	0.8563983739423122	0.5193773182996253	F	F	F
0.9814354254124780	0.1396032612863678	0.4834948480823442	F	F	F
0.4455303170494048	0.1384417431213530	0.6061923914256894	T	T	T
0.1076155153809581	0.8934397921247412	0.6383471403484104	T	T	T
0.9441517550824675	0.3665557919140173	0.6062990013683708	T	T	T
0.1876379429804738	0.3638725973297565	0.6046723848472004	T	T	T
0.3570758608726049	0.6550206040334087	0.6369336950465426	T	T	T
0.8542329598307185	0.8439237236879963	0.6384101430909600	T	T	T
0.6882367432370057	0.1406611061103204	0.6032446195495634	T	T	T
0.6701792720608802	0.1128835710507530	0.7319509244990839	T	T	T
0.9707662159342211	0.8169498773500176	0.3415467258267725	T	T	T
0.7482524263991701	0.1735111898774915	0.4205926242875910	T	T	T
0.2530381852970049	0.3116095307479329	0.4236059283005952	T	T	T

0.4747664484571988	0.6935443911848923	0.3418568822448895	T	T	T
0.8050619716811896	0.6912250195000722	0.3965123502746696	T	T	T
0.9005844670221651	0.3175832976399867	0.3646637743065467	T	T	T
0.4105123356683783	0.1805130900308897	0.3649798590514239	T	T	T
0.3116581155927892	0.8095622852695941	0.3969548403502156	T	T	T
0.0655916637162359	0.4605232277063974	0.3903177712336480	T	T	T
0.6487606435111566	0.5480518340078678	0.3723343365096256	T	T	T
0.1484082863538433	0.9614013910219934	0.3704421270705534	T	T	T
0.5756183855814035	0.0312263936173082	0.3940607068670787	T	T	T
0.7226775209855038	0.0362406597790496	0.3393615729593864	T	T	T
0.9838748733374335	0.9638910593343794	0.4234800224438557	T	T	T
0.4868774120986913	0.5330720782596594	0.4236132297112186	T	T	T
0.2311784349669976	0.4527814172450306	0.3411973725565741	T	T	T
0.6690919997630900	0.8170932275262288	0.4621108699766978	F	F	F
0.4563443067348629	0.1856957460417874	0.5415381954083784	F	F	F
0.9563715435325619	0.3157762323396867	0.5415514049333012	F	F	F
0.1684768759925106	0.6845410757490313	0.4614047933963619	F	F	F
0.5163401794135183	0.6840621747006708	0.5172222351935218	F	F	F
0.6122121268392959	0.3153938228045661	0.4863254931615089	F	F	F
0.1121104352761861	0.1862923125396918	0.4862169103188876	F	F	F
0.0164653504910319	0.8169379209085434	0.5170864510602016	F	F	F
0.7737086930159478	0.4642121896258828	0.5098542901532497	F	F	F
0.3547568199701061	0.5398845750144545	0.4913055491984935	F	F	F
0.8548352112812623	0.9612879754852131	0.4913474116743402	F	F	F
0.2736558171006749	0.0367285287095171	0.5095842622449496	F	F	F
0.4364578605973435	0.0348585244096000	0.4598389770138454	F	F	F
0.6931547229194095	0.9653791778681509	0.5438751113830449	F	F	F
0.1930960752500894	0.5368671613790212	0.5435284188581946	F	F	F
0.9363025789852344	0.4660265976351923	0.4598071447971463	F	F	F

0.3743974293623429	0.8197340950524064	0.5813473373810510	T	T	T
0.1571351612067950	0.1872555789777698	0.6616028470065408	T	T	T
0.6551303535500266	0.3440293158982064	0.6582070318617542	T	T	T
0.8749077382325021	0.6834318502830194	0.5815495551572804	T	T	T
0.2243696615652918	0.6837669942558158	0.6406517123305377	T	T	T
0.3212153782286817	0.3127772099042255	0.6095381996140187	T	T	T
0.8183417906736398	0.1834061775140763	0.6073392429414578	T	T	T
0.7185752952771995	0.8244883540118612	0.6409663285044781	T	T	T
0.4862578663289897	0.4705246120021915	0.6282210310947692	T	T	T
0.0626896688409015	0.5343695996414097	0.6097189882625850	T	T	T
0.5633174959739997	0.9547329261755038	0.6112154903933172	T	T	T
0.9794421960377545	0.0331628624875427	0.6337962180452473	T	T	T
0.1453438396500041	0.0315704857939128	0.5799382374197716	T	T	T
0.4093527392982253	0.9503109542923143	0.6646753744027619	T	T	T
0.9036353125395661	0.5430295487646057	0.6641669546494350	T	T	T
0.6454306158556509	0.4767510136077591	0.5801790806470593	T	T	T
0.0699580936760170	0.6769215896176287	0.6985115131472657	T	T	T
0.3664608355303944	0.4331861450891260	0.7019819193498883	T	T	T
0.8510724379873903	0.0653921360619663	0.7014333356803364	T	T	T
0.5601699694481649	0.7423281404616787	0.6954915818844110	T	T	T
0.2801757210066939	0.9279347174777031	0.3030947455499846	T	T	T
0.5627283705539935	0.1756678848941980	0.3061563897763797	T	T	T
0.7715020340849595	0.5790748433097842	0.3011476058846794	T	T	T
0.0341395968368617	0.3139819964126733	0.3002405427433875	T	T	T
0.0034166600117854	0.6214594625954006	0.6916890691421193	T	T	T
0.3705564926273069	0.2466201854731611	0.6930089558209327	T	T	T
0.8690275701074579	0.2460910548070473	0.6933013503131661	T	T	T
0.6047521580363737	0.8683814217983191	0.7099551614194900	T	T	T
0.1067593012344800	0.5155497701889218	0.6962295595172346	T	T	T

0.4287095370771119	0.4745683916187580	0.7139243353957385	T	T	T
0.7882128158702938	0.0760400080830420	0.7160526969711365	T	T	T
0.5014965863490374	0.8475686575584719	0.6860000397165840	T	T	T
0.2240623922745636	0.9743572497604278	0.2860101481894436	T	T	T
0.2706956221874283	0.7429150279317907	0.3122416076982669	T	T	T
0.5198916167066560	0.0255544959131210	0.3076589531399454	T	T	T
0.6265811839066113	0.1019042146744403	0.3161512777703326	T	T	T
0.7606095874856013	0.7616658579065263	0.3129436730161305	T	T	T
0.7151564336741599	0.5404122956376628	0.2836067633780166	T	T	T
0.0254558992144695	0.4959407823928279	0.3102480642670982	T	T	T
0.9753432420491958	0.2719564472620761	0.2849213830806357	T	T	T
0.6586403673293358	0.2364907576995093	0.7046384662133228	T	T	T
0.6530024493883717	0.2052770294276681	0.7594223530464832	T	T	T
0.6048094563230663	0.6282965905616056	0.6352721465270051	T	T	T
0.2344372928950307	0.3634625181788707	0.4844606095791164	F	F	F
0.6877537009426359	0.8789873182593738	0.3978423170947725	T	T	T

Ti O Ti O Ti O

1.000000000000000

14.2453041077000009 0.0000000000000000 0.0000000000000000

0.0000000000000000 5.1680002212999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 29.4789562224999990

Ti O H Co

21 57 17 3

Selective dynamics

Direct

0.0223000933864524	0.1054033125081290	0.3673196136736956	T	T	T
0.1848205791038577	0.6244873513859209	0.3964233853253900	T	T	T
0.5234439515512030	0.4032600376167220	0.3653283613994076	T	T	T

0.7675452284288676	0.3525145841239918	0.3655742261994024	T	T	T
0.9368188031515564	0.6333314878149832	0.3979021882513821	T	T	T
0.4401298418829456	0.8638773610017157	0.4000089409297594	T	T	T
0.2742090759145905	0.1520221724520387	0.3678339678951289	T	T	T
0.7342005810289152	0.1367530326270341	0.4848529224897646	F	F	F
0.3956158154875027	0.8683481241609385	0.5172283169192724	F	F	F
0.8953822014665107	0.6325289816178099	0.5172296942882255	F	F	F
0.6487817750305567	0.6455289705310605	0.5195024736345744	F	F	F
0.4815241771643173	0.3615968561732217	0.4834047030315531	F	F	F
0.1487325421792534	0.8563983739423122	0.5193773182996253	F	F	F
0.9814354254124780	0.1396032612863678	0.4834948480823442	F	F	F
0.4443476123296877	0.1393975728601230	0.6063233872138916	T	T	T
0.1077587172651967	0.8931784267964504	0.6381448560424049	T	T	T
0.9441603118780149	0.3687772718066917	0.6064656784085819	T	T	T
0.1884053211442499	0.3641619630220314	0.6052476224552528	T	T	T
0.3577714642483851	0.6604552386281692	0.6378014039213551	T	T	T
0.8552463765967236	0.8452280620338912	0.6391537865760336	T	T	T
0.6880692339738911	0.1423465834831514	0.6032529106510364	T	T	T
0.6833686575415036	0.0746733153162954	0.7352177289099761	T	T	T
0.9706538312285221	0.8154708560204638	0.3414849772400487	T	T	T
0.7479764523267475	0.1729095492864100	0.4204305838980822	T	T	T
0.2526684011483405	0.3115047781452353	0.4236167342318257	T	T	T
0.4744528039012175	0.6945792073075268	0.3418048229417081	T	T	T
0.8047968114325601	0.6904441848660493	0.3965554352050475	T	T	T
0.9003665859373426	0.3169735092289591	0.3647570802062811	T	T	T
0.4102905279480027	0.1804437304039332	0.3651211400254578	T	T	T
0.3113274907393406	0.8093080322717551	0.3970265952988839	T	T	T
0.0653791218237174	0.4601294148517722	0.3903310445527721	T	T	T
0.6485060203039208	0.5476079198431943	0.3723256221026033	T	T	T



0.1482237765526234 0.9612055577806963 0.3704189532439663 T T T  
0.5758596061432421 0.0298613220070059 0.3941343618458378 T T T  
0.7225544460695057 0.0357294220425057 0.3393412380996421 T T T  
0.9836743739415920 0.9634213442351859 0.4233577650188907 T T T  
0.4866404725147566 0.5331394776752381 0.4235048348825195 T T T  
0.2311631510406054 0.4528529663013607 0.3412006998635277 T T T  
0.6690919997630900 0.8170932275262288 0.4621108699766978 F F F  
0.4563443067348629 0.1856957460417874 0.5415381954083784 F F F  
0.9563715435325619 0.3157762323396867 0.5415514049333012 F F F  
0.1684768759925106 0.6845410757490313 0.4614047933963619 F F F  
0.5163401794135183 0.6840621747006708 0.5172222351935218 F F F  
0.6122121268392959 0.3153938228045661 0.4863254931615089 F F F  
0.1121104352761861 0.1862923125396918 0.4862169103188876 F F F  
0.0164653504910319 0.8169379209085434 0.5170864510602016 F F F  
0.7737086930159478 0.4642121896258828 0.5098542901532497 F F F  
0.3547568199701061 0.5398845750144545 0.4913055491984935 F F F  
0.8548352112812623 0.9612879754852131 0.4913474116743402 F F F  
0.2736558171006749 0.0367285287095171 0.5095842622449496 F F F  
0.4364578605973435 0.0348585244096000 0.4598389770138454 F F F  
0.6931547229194095 0.9653791778681509 0.5438751113830449 F F F  
0.1930960752500894 0.5368671613790212 0.5435284188581946 F F F  
0.9363025789852344 0.4660265976351923 0.4598071447971463 F F F  
0.3745336373846822 0.8209373748811348 0.5811672560274683 T T T  
0.1577951465825208 0.1871137839160578 0.6614330147806260 T T T  
0.6540890387804984 0.3406445460967472 0.6585808120362766 T T T  
0.8756572121926025 0.6849142136543523 0.5813475699298776 T T T  
0.2247478210797592 0.6844715693871575 0.6411226028436622 T T T  
0.3216006804242075 0.3180056013200532 0.6091836243605900 T T T  
0.8179359372017070 0.1845243260809455 0.6077538319598600 T T T

0.7185488829210785 0.8181649103507639 0.6393468233428194 T T T  
0.4869150677988345 0.4757075703070343 0.6263944251032475 T T T  
0.0632380915855687 0.5353391008741524 0.6097128551520691 T T T  
0.5635133341254354 0.9599779485791655 0.6118506988272018 T T T  
0.9798687217804231 0.0333811251874686 0.6334268983089090 T T T  
0.1461804356887815 0.0315256733016460 0.5797836430058217 T T T  
0.4072229992091785 0.9598112701955476 0.6637840203306309 T T T  
0.9045796019652604 0.5432046502697613 0.6637807935235480 T T T  
0.6457692151964823 0.4774979204056320 0.5798347442819087 T T T  
0.0700631177125779 0.6831015094163944 0.6987780765416695 T T T  
0.3765155299431099 0.4477796765383664 0.7017672953857037 T T T  
0.8490377572707678 0.0490662756326524 0.7010493564162028 T T T  
0.5665496440787104 0.7263346420878443 0.6931997511259760 T T T  
0.2806268191732332 0.9277359981095156 0.3032464174956472 T T T  
0.5623325007696759 0.1752439035347272 0.3063900819333936 T T T  
0.7717368814013853 0.5789381319694948 0.3011965765451676 T T T  
0.0340688886318311 0.3143819275569623 0.3003347186207724 T T T  
0.0037751095206175 0.6250609295273081 0.6924926265028775 T T T  
0.3789377887206082 0.2593900566904073 0.6941538193939527 T T T  
0.8674184036352809 0.2309766362042392 0.6955632050945179 T T T  
0.6473946583596195 0.9208073542708548 0.7248283604045002 T T T  
0.1073799844824608 0.5226188032290863 0.6978803116195351 T T T  
0.4405244747248199 0.4926296625457128 0.7115260977453653 T T T  
0.7837502398797837 0.0517577476316863 0.7167686079943878 T T T  
0.5151589168686986 0.8527599512022783 0.6862888005147177 T T T  
0.2258278478913094 0.9750022767314876 0.2852686895065851 T T T  
0.2704403697151359 0.7427411067261478 0.3122315347803685 T T T  
0.5196303398569716 0.0247711815643907 0.3078147351641600 T T T  
0.6263141472139040 0.1017576360802749 0.3162050029987207 T T T

0.7604272214301415	0.7615247683722337	0.3128756715295859	T	T	T
0.7164404823946920	0.5402685530562850	0.2828934208016751	T	T	T
0.0241989104605318	0.4961514417547639	0.3102394585614106	T	T	T
0.9766712569212554	0.2709257165795390	0.2839529579094429	T	T	T
0.6624763733791603	0.2099695530371246	0.7135010636453983	T	T	T
0.6048518494500329	0.6286992664713308	0.6365350223746713	T	T	T
0.2344372928950307	0.3634625181788707	0.4844606095791164	F	F	F
0.6875307072902441	0.8784428752747826	0.3979791636360009	T	T	T

Ti O H Co

1.0000000000000000		
14.2453041077000009	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.1680002212999998	0.0000000000000000
0.0000000000000000	0.0000000000000000	29.4789562224999990

Ti O H Co

21 57 17 3

Selective dynamics

Direct

0.0241387915228473	0.1093337193648202	0.3679833960494572	T	T	T
0.1868717400385466	0.6249923954595964	0.3965986814185572	T	T	T
0.5252965494326874	0.3988064031554456	0.3660522787539420	T	T	T
0.7680024234918681	0.3542440847366420	0.3660227270418956	T	T	T
0.9374863247852807	0.6362395693451571	0.3969292504682205	T	T	T
0.4424050228649126	0.8632913276318609	0.3989966656415271	T	T	T
0.2751003934621680	0.1520235131165981	0.3681498021694400	T	T	T
0.7342005810289152	0.1367530326270341	0.4848529224897646	F	F	F
0.3956158154875027	0.8683481241609385	0.5172283169192724	F	F	F
0.8953822014665107	0.6325289816178099	0.5172296942882255	F	F	F
0.6487817750305567	0.6455289705310605	0.5195024736345744	F	F	F

0.4815241771643173 0.3615968561732217 0.4834047030315531 F F F  
0.1487325421792534 0.8563983739423122 0.5193773182996253 F F F  
0.9814354254124780 0.1396032612863678 0.4834948480823442 F F F  
0.4493751672017812 0.1442286547201976 0.6052042550498148 T T T  
0.1072269842909131 0.9011240722627545 0.6392745087912202 T T T  
0.9434188856155024 0.3718090976633286 0.6058005891926385 T T T  
0.1842119472583668 0.3687544135806025 0.6034158375929071 T T T  
0.3544421824231853 0.6405046114277788 0.6353250917976496 T T T  
0.8541614144155373 0.8502939400588457 0.6382979052661631 T T T  
0.6893021544912725 0.1421504047769831 0.6009566898923759 T T T  
0.6140620423868941 0.9247655576527846 0.7193948247385210 T T T  
0.9712041866820217 0.8192208687698692 0.3416996618912105 T T T  
0.7484265440401704 0.1754285592094838 0.4210433359137666 T T T  
0.2534437519976169 0.3114376182409511 0.4237067427598794 T T T  
0.4751319972875339 0.6907364150349846 0.3421471604887837 T T T  
0.8056471377708349 0.6930286485272877 0.3964094650761616 T T T  
0.9009026655597959 0.3182634567069098 0.3647822301475271 T T T  
0.4109498219664801 0.1810698746491177 0.3649005386416471 T T T  
0.3122623656381883 0.8098564068863454 0.3968871605037926 T T T  
0.0659883558677763 0.4610248082838661 0.3903014541287378 T T T  
0.6492832905172002 0.5492578324516205 0.3724477330678942 T T T  
0.1487508708542221 0.9618742198748348 0.3706482183360390 T T T  
0.5751763260385021 0.0338514735540584 0.3939237359036305 T T T  
0.7230415033690544 0.0377073302999788 0.3395216675585133 T T T  
0.9842034081571807 0.9650106011972408 0.4237289286070980 T T T  
0.4875014916915748 0.5329156128335099 0.4240186612142311 T T T  
0.2314226163511390 0.4526524338845186 0.3412967602624632 T T T  
0.6690919997630900 0.8170932275262288 0.4621108699766978 F F F  
0.4563443067348629 0.1856957460417874 0.5415381954083784 F F F

0.9563715435325619 0.3157762323396867 0.5415514049333012 F F F  
0.1684768759925106 0.6845410757490313 0.4614047933963619 F F F  
0.5163401794135183 0.6840621747006708 0.5172222351935218 F F F  
0.6122121268392959 0.3153938228045661 0.4863254931615089 F F F  
0.1121104352761861 0.1862923125396918 0.4862169103188876 F F F  
0.0164653504910319 0.8169379209085434 0.5170864510602016 F F F  
0.7737086930159478 0.4642121896258828 0.5098542901532497 F F F  
0.3547568199701061 0.5398845750144545 0.4913055491984935 F F F  
0.8548352112812623 0.9612879754852131 0.4913474116743402 F F F  
0.2736558171006749 0.0367285287095171 0.5095842622449496 F F F  
0.4364578605973435 0.0348585244096000 0.4598389770138454 F F F  
0.6931547229194095 0.9653791778681509 0.5438751113830449 F F F  
0.1930960752500894 0.5368671613790212 0.5435284188581946 F F F  
0.9363025789852344 0.4660265976351923 0.4598071447971463 F F F  
0.3755207508898955 0.8233484873116547 0.5825459948252306 T T T  
0.1568932751041648 0.1932395946270679 0.6619784202596727 T T T  
0.6622644846712530 0.3358625784718652 0.6622254014974551 T T T  
0.8752146642616577 0.6876731658631563 0.5818162590016446 T T T  
0.2239901148236323 0.6885441273528485 0.6400385604931226 T T T  
0.3212002310149202 0.3120740041392402 0.6099671186710680 T T T  
0.8182312979047205 0.1899864054096312 0.6057081491585525 T T T  
0.7198942352062957 0.8272095998096629 0.6408155583867623 T T T  
0.4859849410724181 0.4660434804829246 0.6313292385530265 T T T  
0.0623840913510043 0.5387763535059614 0.6095575674256433 T T T  
0.5631130384072198 0.9553134332517027 0.6123640022489841 T T T  
0.9783766039631019 0.0427454860962840 0.6357775657489103 T T T  
0.1434467652071169 0.0357926967678780 0.5804112434928337 T T T  
0.4082929304502576 0.9562504168771551 0.6670353582540001 T T T  
0.9054148066517380 0.5558266653858955 0.6646242431589133 T T T

0.6452656019265792	0.4751386269865681	0.5811760900554753	T	T	T
0.0710373199424914	0.6787964706540091	0.6984868666007306	T	T	T
0.3589022758733636	0.4405878796715174	0.7026478636130937	T	T	T
0.8292679266222374	0.1102581718879372	0.6984159935162260	T	T	T
0.5627773720370884	0.7260812306361806	0.6950558245836298	T	T	T
0.2805208072503729	0.9281630421624999	0.3031519605506265	T	T	T
0.5637914308634339	0.1793729065490375	0.3057167730898699	T	T	T
0.7720560502755113	0.5794903549457583	0.3013449862376976	T	T	T
0.0347675492827544	0.3121568422184011	0.3002558477769650	T	T	T
0.0045677540276298	0.6227691883281867	0.6910814111358996	T	T	T
0.3662622155376808	0.2536270253032574	0.6947521395213324	T	T	T
0.8732853228242166	0.2585393979196197	0.6948879964686356	T	T	T
0.1084349307375986	0.5183117468787192	0.6960315319712781	T	T	T
0.4174310879706062	0.4879384998625023	0.7177828623522314	T	T	T
0.7692727821546587	0.1960720480707930	0.6899867833469100	T	T	T
0.4675935476686181	0.8927518471366463	0.6819420064365601	T	T	T
0.2245878611108032	0.9749786345441737	0.2859668681462598	T	T	T
0.2709705641065567	0.7430518454417009	0.3122009805005617	T	T	T
0.5203536580662252	0.0308293169772292	0.3063891194713210	T	T	T
0.6271007655674555	0.1032342997235467	0.3159298292221595	T	T	T
0.7611453061040313	0.7621641165490363	0.3130169147757090	T	T	T
0.7157613409418914	0.5402227918308448	0.2838070877597115	T	T	T
0.0267256012821097	0.4947309938836567	0.3099001489721669	T	T	T
0.9757032900810134	0.2698723689643557	0.2852081196657809	T	T	T
0.6182337963011647	0.2373791551771895	0.6813107698417967	T	T	T
0.6786621550243840	0.8572496081027200	0.7183033644171646	T	T	T
0.6053358396412557	0.6383153397846391	0.6372140055334967	T	T	T
0.2344372928950307	0.3634625181788707	0.4844606095791164	F	F	F
0.6883856422770585	0.8804361834767056	0.3975441773708069	T	T	T

Ti O H Co

1.0000000000000000

14.2453041077000009 0.0000000000000000 0.0000000000000000

0.0000000000000000 5.1680002212999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 29.4789562224999990

Ti O H Co

21 57 16 3

Selective dynamics

Direct

0.0236297539373734 0.1083757763361208 0.3677902959031907 T T T

0.1863046334708358 0.6249087097404273 0.3964982584735083 T T T

0.5249808685121041 0.3994894149055478 0.3659531805372439 T T T

0.7678697172129305 0.3538493434495144 0.3658869279648793 T T T

0.9372401573284336 0.6356000755760496 0.3972207661069340 T T T

0.4419421742422560 0.8632294833719033 0.3991543445600079 T T T

0.2749110476994686 0.1519808133017997 0.3680879914082023 T T T

0.7342005810289152 0.1367530326270341 0.4848529224897646 F F F

0.3956158154875027 0.8683481241609385 0.5172283169192724 F F F

0.8953822014665107 0.6325289816178099 0.5172296942882255 F F F

0.6487817750305567 0.6455289705310605 0.5195024736345744 F F F

0.4815241771643173 0.3615968561732217 0.4834047030315531 F F F

0.1487325421792534 0.8563983739423122 0.5193773182996253 F F F

0.9814354254124780 0.1396032612863678 0.4834948480823442 F F F

0.4499090485217088 0.1466837421021597 0.6052695963594760 T T T

0.1071015246427987 0.8996548571624903 0.6389030397623272 T T T

0.9434850984974748 0.3709559686610954 0.6057986695833782 T T T

0.1845766583534148 0.3684892831001857 0.6037578453611456 T T T

0.3550843266161025 0.6424545817816457 0.6354748901391177 T T T

0.8541071587477674 0.8486348550568282 0.6386264797713537 T T T

0.6897068352938903	0.1436902845603353	0.6011403039370645	T	T	T
0.5633339930431592	0.9516816737890563	0.7121352460614573	T	T	T
0.9710700677786035	0.8184322440158441	0.3416462601283792	T	T	T
0.7482967194139005	0.1750569657864630	0.4208927542628901	T	T	T
0.2533635636998317	0.3116730193169123	0.4236822189607918	T	T	T
0.4750339123680087	0.6913518458315332	0.3421108207819377	T	T	T
0.8054621070402961	0.6928348652758042	0.3964477526720684	T	T	T
0.9007722368109978	0.3181241120524587	0.3647720645007143	T	T	T
0.4108340917379146	0.1809281909849498	0.3649591595250233	T	T	T
0.3120880251087902	0.8098801336514457	0.3969088577446456	T	T	T
0.0658330241575384	0.4610437952248865	0.3902999950610739	T	T	T
0.6490716615911484	0.5488914894097835	0.3725136796037990	T	T	T
0.1486460790303319	0.9618199847236328	0.3705818502919980	T	T	T
0.5753135804749715	0.0331042304820433	0.3939823702877689	T	T	T
0.7229286142880269	0.0375920539140433	0.3394478282278420	T	T	T
0.9841190714377300	0.9647308866821086	0.4236337246641503	T	T	T
0.4872162493922436	0.5328549069547075	0.4239381973142177	T	T	T
0.2313887685906802	0.4527769739393094	0.3412843816804930	T	T	T
0.6690919997630900	0.8170932275262288	0.4621108699766978	F	F	F
0.4563443067348629	0.1856957460417874	0.5415381954083784	F	F	F
0.9563715435325619	0.3157762323396867	0.5415514049333012	F	F	F
0.1684768759925106	0.6845410757490313	0.4614047933963619	F	F	F
0.5163401794135183	0.6840621747006708	0.5172222351935218	F	F	F
0.6122121268392959	0.3153938228045661	0.4863254931615089	F	F	F
0.1121104352761861	0.1862923125396918	0.4862169103188876	F	F	F
0.0164653504910319	0.8169379209085434	0.5170864510602016	F	F	F
0.7737086930159478	0.4642121896258828	0.5098542901532497	F	F	F
0.3547568199701061	0.5398845750144545	0.4913055491984935	F	F	F
0.8548352112812623	0.9612879754852131	0.4913474116743402	F	F	F



0.2736558171006749 0.0367285287095171 0.5095842622449496 F F F  
0.4364578605973435 0.0348585244096000 0.4598389770138454 F F F  
0.6931547229194095 0.9653791778681509 0.5438751113830449 F F F  
0.1930960752500894 0.5368671613790212 0.5435284188581946 F F F  
0.9363025789852344 0.4660265976351923 0.4598071447971463 F F F  
0.3763036712490866 0.8257594798052655 0.5826740771139085 T T T  
0.1578851949555375 0.1915410062787463 0.6617019929748260 T T T  
0.6602639863273188 0.3298954333084532 0.6620718520253399 T T T  
0.8759149251105161 0.6875383920825596 0.5816375918972411 T T T  
0.2240652803727337 0.6882312343069266 0.6397724756154813 T T T  
0.3216603088493861 0.3175688933481697 0.6090602080547786 T T T  
0.8184587349013303 0.1893978332008568 0.6058199986690558 T T T  
0.7206418324927960 0.8245283852055515 0.6398713318546574 T T T  
0.4855152914315982 0.4676106208710571 0.6324345921043036 T T T  
0.0626642289497895 0.5384253644035584 0.6095452336701555 T T T  
0.5621145161220709 0.9560386020313028 0.6139947872450426 T T T  
0.9790561321194179 0.0406107568006876 0.6351002807973696 T T T  
0.1439752187527046 0.0353799292291789 0.5801225777128044 T T T  
0.4015470171558777 0.9681414157814002 0.6668832008496851 T T T  
0.9048700371780275 0.5507983482444190 0.6643232760918968 T T T  
0.6443663074133944 0.4716990316117629 0.5803430450684897 T T T  
0.0709773668382600 0.6797897572915735 0.6984829415972462 T T T  
0.3523133373051548 0.4450879990294824 0.7026531301398655 T T T  
0.8376322928922806 0.0971511078928292 0.6989563522888387 T T T  
0.5813041588273841 0.7137484614910883 0.6983939593109426 T T T  
0.2806521945669589 0.9281260532228023 0.3031507682134982 T T T  
0.5634201172906966 0.1786907350476920 0.3058365721427337 T T T  
0.7717896927335487 0.5797128404840522 0.3013336456010527 T T T  
0.0346052951829627 0.3131164078890978 0.3002975626476179 T T T

0.0045704363682336	0.6225884751751949	0.6916060446636554	T	T	T
0.3546894259631092	0.2582454744441527	0.6938784595628611	T	T	T
0.8686944123944823	0.2662614700929850	0.6916906306885369	T	T	T
0.1084877514702208	0.5195464928806027	0.6965008462291125	T	T	T
0.4102131232543046	0.4764097503181161	0.7194329162691158	T	T	T
0.7708673352763444	0.1446950580475151	0.6993903088428292	T	T	T
0.4579546389912101	0.9617777295062829	0.6867446583333948	T	T	T
0.2249980671811156	0.9746939324368081	0.2857312095728849	T	T	T
0.2709871070223930	0.7430591195169729	0.3122019402245677	T	T	T
0.5200961939674396	0.0298169102537509	0.3066236755734200	T	T	T
0.6268511656498583	0.1030093466127514	0.3159597545628606	T	T	T
0.7607917263139224	0.7623898247981844	0.3130081554225327	T	T	T
0.7157238948378660	0.5405518890495409	0.2836211544533914	T	T	T
0.0260364602888135	0.4954518590245665	0.3100299962058487	T	T	T
0.9759884338427236	0.2704755294654397	0.2848767667861210	T	T	T
0.6135094466962608	0.2267195569579017	0.6791863961373299	T	T	T
0.6060981893607245	0.6374999246066946	0.6384534584987641	T	T	T
0.2344372928950307	0.3634625181788707	0.4844606095791164	F	F	F
0.6881857810252252	0.8802019929030630	0.3976959456962538	T	T	T

Ti O H Co

1.0000000000000000

14.2453041077000009 0.0000000000000000 0.0000000000000000

0.0000000000000000 5.1680002212999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 29.4789562224999990

Ti O H Co

21 57 15 3

Selective dynamics

Direct

0.0227696827981051 0.1068561659624472 0.3675376091299133 T T T  
0.1854033708675458 0.6248045693642812 0.3964627751145398 T T T  
0.5238067655647053 0.4024919237025220 0.3654743997611511 T T T  
0.7675127977231948 0.3534594607393276 0.3657810374313846 T T T  
0.9369277494000735 0.6344278188457997 0.3975953696814883 T T T  
0.4407612984800735 0.8640956752324094 0.3998235435864008 T T T  
0.2744340319936093 0.1521610727551697 0.3679001481683468 T T T  
0.7342005810289152 0.1367530326270341 0.4848529224897646 F F F  
0.3956158154875027 0.8683481241609385 0.5172283169192724 F F F  
0.8953822014665107 0.6325289816178099 0.5172296942882255 F F F  
0.6487817750305567 0.6455289705310605 0.5195024736345744 F F F  
0.4815241771643173 0.3615968561732217 0.4834047030315531 F F F  
0.1487325421792534 0.8563983739423122 0.5193773182996253 F F F  
0.9814354254124780 0.1396032612863678 0.4834948480823442 F F F  
0.4394301178143830 0.1476018058940461 0.6066481436161342 T T T  
0.1091317347128687 0.8969717002870760 0.6383437136875985 T T T  
0.9451095908538719 0.3705137364178632 0.6062227080433146 T T T  
0.1872351899329391 0.3693944020924479 0.6046473182823247 T T T  
0.3595726467466911 0.6636006719350714 0.6382660313132705 T T T  
0.8546345909061631 0.8491973704775490 0.6380247940482849 T T T  
0.6900890955214833 0.1446065598894150 0.6013950987244036 T T T  
0.5868880336182325 0.9414971100779642 0.7151047982025499 T T T  
0.9706915435792385 0.8169929467712973 0.3415477173838214 T T T  
0.7480745683021449 0.1740937285275617 0.4206907275458864 T T T  
0.2528934191222554 0.3115579175944065 0.4236260912720301 T T T  
0.4746661107983035 0.6941149096043454 0.3418571676041136 T T T  
0.8049751668835260 0.6916721449214047 0.3964875848188483 T T T  
0.9003891273286464 0.3177065158480083 0.3647468019626440 T T T  
0.4103466175242423 0.1809152875275486 0.3650298706115202 T T T

0.3115129838038695	0.8096375404525946	0.3969292046775643	T	T	T
0.0654748794047099	0.4606978238838566	0.3903220828741632	T	T	T
0.6486571780001121	0.5485593845750024	0.3723497446251674	T	T	T
0.1482663001437215	0.9615665942946113	0.3704987822979132	T	T	T
0.5755483763229565	0.0314935037486880	0.3940823945511833	T	T	T
0.7225252503791462	0.0366876070020131	0.3394465956845873	T	T	T
0.9837134565582178	0.9642052714086481	0.4234749908712306	T	T	T
0.4868167247435508	0.5333678872904934	0.4235918308753618	T	T	T
0.2310375833307609	0.4528539617767003	0.3411932494239641	T	T	T
0.6690919997630900	0.8170932275262288	0.4621108699766978	F	F	F
0.4563443067348629	0.1856957460417874	0.5415381954083784	F	F	F
0.9563715435325619	0.3157762323396867	0.5415514049333012	F	F	F
0.1684768759925106	0.6845410757490313	0.4614047933963619	F	F	F
0.5163401794135183	0.6840621747006708	0.5172222351935218	F	F	F
0.6122121268392959	0.3153938228045661	0.4863254931615089	F	F	F
0.1121104352761861	0.1862923125396918	0.4862169103188876	F	F	F
0.0164653504910319	0.8169379209085434	0.5170864510602016	F	F	F
0.7737086930159478	0.4642121896258828	0.5098542901532497	F	F	F
0.3547568199701061	0.5398845750144545	0.4913055491984935	F	F	F
0.8548352112812623	0.9612879754852131	0.4913474116743402	F	F	F
0.2736558171006749	0.0367285287095171	0.5095842622449496	F	F	F
0.4364578605973435	0.0348585244096000	0.4598389770138454	F	F	F
0.6931547229194095	0.9653791778681509	0.5438751113830449	F	F	F
0.1930960752500894	0.5368671613790212	0.5435284188581946	F	F	F
0.9363025789852344	0.4660265976351923	0.4598071447971463	F	F	F
0.3766364786254501	0.8169017170390933	0.5811761536576479	T	T	T
0.1578606690123748	0.1910207319122854	0.6615451709833262	T	T	T
0.6577436104327228	0.3428636196400804	0.6611858337353521	T	T	T
0.8753109106024726	0.6880063779365313	0.5813222835388743	T	T	T

0.2240931525980686	0.6857973473551962	0.6401481415685901	T	T	T
0.3199382165390475	0.3177086970599040	0.6074609585238787	T	T	T
0.8181784699608536	0.1909394130688938	0.6059025308285311	T	T	T
0.7194128987718580	0.8303662856006084	0.6399689779982081	T	T	T
0.4854547429590872	0.4705564944744119	0.6306889969688138	T	T	T
0.0621410811946831	0.5397718516912606	0.6095356257382704	T	T	T
0.5631115519453065	0.9549818166350076	0.6131859365801924	T	T	T
0.9786556787115587	0.0398281475558302	0.6347317762930719	T	T	T
0.1442971960645709	0.0345427206080949	0.5797811158956964	T	T	T
0.4004271849063528	0.9670005584344494	0.6633812773625486	T	T	T
0.9037227833680666	0.5502422776455029	0.6641302114920726	T	T	T
0.6453027538491471	0.4757200399567285	0.5799803121521923	T	T	T
0.0703208851988546	0.6829625254840502	0.6985963034831547	T	T	T
0.3575627888153558	0.4367920354812415	0.7019178711947093	T	T	T
0.8385698334104611	0.0928033883577850	0.6992463484344124	T	T	T
0.5698670543321126	0.7189451355630097	0.6978431090578454	T	T	T
0.2802059514308606	0.9280964435117103	0.3031477800331668	T	T	T
0.5625408613133356	0.1762111013282322	0.3061664122649579	T	T	T
0.7714673418191295	0.5791154940903809	0.3011899474984008	T	T	T
0.0339501118174440	0.3142285009811668	0.3002943683577995	T	T	T
0.0040604574813109	0.6259381647543727	0.6918061232979710	T	T	T
0.3659375307184253	0.2504661350676280	0.6930940486961068	T	T	T
0.8649587494010437	0.2671756815784552	0.6913933967119361	T	T	T
0.1076355402594673	0.5223593828321711	0.6971511273343182	T	T	T
0.4134059107177908	0.4815135937417135	0.7193990565510882	T	T	T
0.7710952026661729	0.1250234548764632	0.7022063311136953	T	T	T
0.2247969427491542	0.9751839869983637	0.2855899401281585	T	T	T
0.2703238704353313	0.7430579587824349	0.3121834428690122	T	T	T
0.5196574411210956	0.0261651851296742	0.3075419710366872	T	T	T

0.6263337258967445	0.1022565898313180	0.3161396713566093	T	T	T
0.7604095896651674	0.7616621427471990	0.3128948023356684	T	T	T
0.7155253906450455	0.5401692196774587	0.2833670485160877	T	T	T
0.0249200700748000	0.4962334885855726	0.3102003048363848	T	T	T
0.9756244811914064	0.2716164490187341	0.2846096917888158	T	T	T
0.6115572880879893	0.2414886369300918	0.6787386760671384	T	T	T
0.6036411688656224	0.6461807161385719	0.6353625572673588	T	T	T
0.2344372928950307	0.3634625181788707	0.4844606095791164	F	F	F
0.6877017421825278	0.8794958889817803	0.3977750442782648	T	T	T

Ti O H Co

1.000000000000000

14.2453041077000009 0.0000000000000000 0.0000000000000000

0.0000000000000000 5.1680002212999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 29.4789562224999990

Ti O H Co

21 55 15 3

Selective dynamics

Direct

0.0239376696324027	0.1093076606831801	0.3679683539305217	T	T	T
0.1867363990701935	0.6255185523269507	0.3965889299559912	T	T	T
0.5248051060540877	0.4003363233019220	0.3659223641513337	T	T	T
0.7677573546017917	0.3546048180536873	0.3660412774837095	T	T	T
0.9373862854675101	0.6361722843090691	0.3969114649137576	T	T	T
0.4421021645064444	0.8642147446916835	0.3992590156340144	T	T	T
0.2749791098952122	0.1527297851998279	0.3680257654570737	T	T	T
0.7342005810289152	0.1367530326270341	0.4848529224897646	F	F	F
0.3956158154875027	0.8683481241609385	0.5172283169192724	F	F	F
0.8953822014665107	0.6325289816178099	0.5172296942882255	F	F	F

0.6487817750305567 0.6455289705310605 0.5195024736345744 F F F  
0.4815241771643173 0.3615968561732217 0.4834047030315531 F F F  
0.1487325421792534 0.8563983739423122 0.5193773182996253 F F F  
0.9814354254124780 0.1396032612863678 0.4834948480823442 F F F  
0.4413939718690535 0.1423001011591682 0.6062227508648803 T T T  
0.1111524079358935 0.8978023763002327 0.6387900997294390 T T T  
0.9465477888131487 0.3696145815465585 0.6059947250003718 T T T  
0.1888723891537747 0.3693624100002929 0.6038638693388098 T T T  
0.3607725959881691 0.6620054936754983 0.6386554677973135 T T T  
0.8574139635701911 0.8469271203220069 0.6385418353336847 T T T  
0.6910300300498595 0.1279340132250372 0.6021447595341436 T T T  
0.9710363904845588 0.8191875070532322 0.3416539930063905 T T T  
0.7483060539242804 0.1756088787667330 0.4210733927770063 T T T  
0.2533675462417050 0.3120064630131874 0.4236134618194713 T T T  
0.4750420797682983 0.6922584880831266 0.3420843381763947 T T T  
0.8054963274428085 0.6930882171242385 0.3963434646566464 T T T  
0.9006792868443738 0.3183014899514043 0.3647338157138086 T T T  
0.4107578456865825 0.1816294352542548 0.3648774081024613 T T T  
0.3120710737190326 0.8105111974703617 0.3968786989488953 T T T  
0.0658634094829601 0.4611709629474421 0.3902708098743126 T T T  
0.6491151509455795 0.5496668811980453 0.3723881118116056 T T T  
0.1486136993375196 0.9623035436630378 0.3706071960556282 T T T  
0.5751382168948012 0.0341635193759490 0.3939228105893949 T T T  
0.7226854597777052 0.0378011883394670 0.3395429979457442 T T T  
0.9840548976262984 0.9648423607232017 0.4236747718688794 T T T  
0.4873879555026868 0.5335174971932665 0.4239189968902583 T T T  
0.2313714611117102 0.4534387205904731 0.3412199341512079 T T T  
0.6690919997630900 0.8170932275262288 0.4621108699766978 F F F  
0.4563443067348629 0.1856957460417874 0.5415381954083784 F F F

0.9563715435325619	0.3157762323396867	0.5415514049333012	F	F	F
0.1684768759925106	0.6845410757490313	0.4614047933963619	F	F	F
0.5163401794135183	0.6840621747006708	0.5172222351935218	F	F	F
0.6122121268392959	0.3153938228045661	0.4863254931615089	F	F	F
0.1121104352761861	0.1862923125396918	0.4862169103188876	F	F	F
0.0164653504910319	0.8169379209085434	0.5170864510602016	F	F	F
0.7737086930159478	0.4642121896258828	0.5098542901532497	F	F	F
0.3547568199701061	0.5398845750144545	0.4913055491984935	F	F	F
0.8548352112812623	0.9612879754852131	0.4913474116743402	F	F	F
0.2736558171006749	0.0367285287095171	0.5095842622449496	F	F	F
0.4364578605973435	0.0348585244096000	0.4598389770138454	F	F	F
0.6931547229194095	0.9653791778681509	0.5438751113830449	F	F	F
0.1930960752500894	0.5368671613790212	0.5435284188581946	F	F	F
0.9363025789852344	0.4660265976351923	0.4598071447971463	F	F	F
0.3780519661048373	0.8160426950065496	0.5819052851875701	T	T	T
0.1581700855541734	0.1924564578901514	0.6618319828802298	T	T	T
0.6530003959779629	0.3404498856362025	0.6623965541761612	T	T	T
0.8753436702322225	0.6866830264307717	0.5819554133126635	T	T	T
0.2251983514408424	0.6864203102922311	0.6398384998794779	T	T	T
0.3212029576358832	0.3145285334043817	0.6082736947043098	T	T	T
0.8175759589138135	0.1902613187228140	0.6068938882128956	T	T	T
0.7186842608468970	0.8213387236163692	0.6405256991792136	T	T	T
0.4875094846326887	0.4692427107064507	0.6320551801887043	T	T	T
0.0624915304617042	0.5380406538276338	0.6097565379612916	T	T	T
0.5627621648370930	0.9556184836059489	0.6137465013356109	T	T	T
0.9787074353368165	0.0386100882364797	0.6352976443393483	T	T	T
0.1443590100547797	0.0352763571776196	0.5801330499395086	T	T	T
0.4029104875623373	0.9611870684987480	0.6648083280487121	T	T	T
0.9051110558166379	0.5495760087542898	0.6648754480933960	T	T	T



0.6450190652740301	0.4673632862914966	0.5807180550446861	T	T	T
0.0729375770134703	0.6775463677775124	0.6986475595456547	T	T	T
0.3525458360641017	0.4231393363386055	0.7012426223407402	T	T	T
0.8344068314473742	0.0978735228102576	0.6990516119963447	T	T	T
0.2800298138065905	0.9285772157230329	0.3031005236775011	T	T	T
0.5633036183807654	0.1797263906770962	0.3056943937605878	T	T	T
0.7711989953354071	0.5788728524794130	0.3011762454204395	T	T	T
0.0345359939288181	0.3125686686965682	0.3002945964102188	T	T	T
0.0064190117292564	0.6225435512012011	0.6920456038149997	T	T	T
0.3642543048275917	0.2378995579248433	0.6919507775015846	T	T	T
0.8661506632883634	0.2661977600598887	0.6917403655787157	T	T	T
0.1096970459058665	0.5160830122903881	0.6958739253797154	T	T	T
0.4007469038447836	0.4660722045945613	0.7233561444930173	T	T	T
0.7676976727993818	0.1452185323982627	0.6979747115922136	T	T	T
0.2238602027392526	0.9756211085382486	0.2861068823634374	T	T	T
0.2703914169359917	0.7436534764882441	0.3122663672260692	T	T	T
0.5197759312352154	0.0313238797782310	0.3065471549971938	T	T	T
0.6265528879936522	0.1035616292681012	0.3159097297408055	T	T	T
0.7605138497420990	0.7615208586321134	0.3128677141315683	T	T	T
0.7144749213978355	0.5395860351453682	0.2839529069701827	T	T	T
0.0266753637558999	0.4950856419209295	0.3100340429500706	T	T	T
0.9752268191631980	0.2707747867280635	0.2854229654410011	T	T	T
0.5955628511023130	0.2510370893071796	0.6719161000670274	T	T	T
0.6056647695587443	0.6346405257051888	0.6310519690197091	T	T	T
0.2344372928950307	0.3634625181788707	0.4844606095791164	F	F	F
0.6881661973940620	0.8807438085058612	0.3974286953494216	T	T	T

Ti O H Co

1.0000000000000000

14.2453041077000009 0.0000000000000000 0.0000000000000000  
0.0000000000000000 5.1680002212999998 0.0000000000000000  
0.0000000000000000 0.0000000000000000 29.4789562224999990

Ti O H Co

21 55 14 3

Selective dynamics

Direct

0.0230196775031099 0.1074695854500471 0.3676278956077701 T T T  
0.1856460095609066 0.6251703819469082 0.3964250898812576 T T T  
0.5240592808752740 0.4026694498592502 0.3655509220542741 T T T  
0.7676310246393220 0.3535527121922862 0.3657995332116458 T T T  
0.9369699221049734 0.6350232981342493 0.3974817475075055 T T T  
0.4409749209719224 0.8642918835558070 0.3998020251488515 T T T  
0.2746860110011534 0.1526006940810605 0.3679476530010400 T T T  
0.7342005810289152 0.1367530326270341 0.4848529224897646 F F F  
0.3956158154875027 0.8683481241609385 0.5172283169192724 F F F  
0.8953822014665107 0.6325289816178099 0.5172296942882255 F F F  
0.6487817750305567 0.6455289705310605 0.5195024736345744 F F F  
0.4815241771643173 0.3615968561732217 0.4834047030315531 F F F  
0.1487325421792534 0.8563983739423122 0.5193773182996253 F F F  
0.9814354254124780 0.1396032612863678 0.4834948480823442 F F F  
0.4407801092463054 0.1441649087820053 0.6068458975472214 T T T  
0.1098532868275756 0.8958059107595955 0.6383291984607502 T T T  
0.9450163729283386 0.3700918747656359 0.6061948596049723 T T T  
0.1879471844282764 0.3685629876734107 0.6044433617820812 T T T  
0.3602685841646539 0.6616126633981740 0.6382608768918034 T T T  
0.8559372613763104 0.8494970746463373 0.6381851033087558 T T T  
0.6884093035714779 0.1386443331498983 0.6022868251287823 T T T  
0.9707911790627429 0.8176776749551031 0.3415754595075618 T T T

0.7483423898877715	0.1744374274130742	0.4207316111259564	T	T	T
0.2530674470857976	0.3119745864887172	0.4236336975887460	T	T	T
0.4748572156054278	0.6941360952382825	0.3418701160620249	T	T	T
0.8051753254763379	0.6920978030527771	0.3965165237630418	T	T	T
0.9005778956390037	0.3181983586164863	0.3646948941232370	T	T	T
0.4105521005278880	0.1811033566200506	0.3649989083567539	T	T	T
0.3116574069921494	0.8100798850130203	0.3969313766437126	T	T	T
0.0656311064884634	0.4610747748711103	0.3902972892865097	T	T	T
0.6488040737678252	0.5486134504392680	0.3724662232174393	T	T	T
0.1484228462050814	0.9620007506973850	0.3704710519098011	T	T	T
0.5756638304147084	0.0317643293303086	0.3941066603449300	T	T	T
0.7226985031493777	0.0371147164419246	0.3394350050888251	T	T	T
0.9839051381588897	0.9645391396622598	0.4235191067689396	T	T	T
0.4868082128189981	0.5335657941554027	0.4236101627354318	T	T	T
0.2312373386283255	0.4533206701514014	0.3412159240174897	T	T	T
0.6690919997630900	0.8170932275262288	0.4621108699766978	F	F	F
0.4563443067348629	0.1856957460417874	0.5415381954083784	F	F	F
0.9563715435325619	0.3157762323396867	0.5415514049333012	F	F	F
0.1684768759925106	0.6845410757490313	0.4614047933963619	F	F	F
0.5163401794135183	0.6840621747006708	0.5172222351935218	F	F	F
0.6122121268392959	0.3153938228045661	0.4863254931615089	F	F	F
0.1121104352761861	0.1862923125396918	0.4862169103188876	F	F	F
0.0164653504910319	0.8169379209085434	0.5170864510602016	F	F	F
0.7737086930159478	0.4642121896258828	0.5098542901532497	F	F	F
0.3547568199701061	0.5398845750144545	0.4913055491984935	F	F	F
0.8548352112812623	0.9612879754852131	0.4913474116743402	F	F	F
0.2736558171006749	0.0367285287095171	0.5095842622449496	F	F	F
0.4364578605973435	0.0348585244096000	0.4598389770138454	F	F	F
0.6931547229194095	0.9653791778681509	0.5438751113830449	F	F	F

0.1930960752500894 0.5368671613790212 0.5435284188581946 F F F  
0.9363025789852344 0.4660265976351923 0.4598071447971463 F F F  
0.3764648459254757 0.8176082523052052 0.5814014882514271 T T T  
0.1577972380467601 0.1903755303300991 0.6615407620606969 T T T  
0.6534586439077753 0.3684274320951149 0.6600326435759836 T T T  
0.8746256912013778 0.6880144056516054 0.5816109791514434 T T T  
0.2241867539643552 0.6849014110944769 0.6398504587277081 T T T  
0.3204081563762009 0.3140134554657353 0.6077780225414252 T T T  
0.8166701102305451 0.1918061016265848 0.6068728491629233 T T T  
0.7195669055498817 0.8339205827587399 0.6421867081295975 T T T  
0.4842195792995637 0.4714811393523705 0.6311709858352667 T T T  
0.0618528109464748 0.5382607262149287 0.6095677929742670 T T T  
0.5629298715647328 0.9479906619398606 0.6148188608222499 T T T  
0.9785732364261405 0.0397620110175312 0.6347397753317515 T T T  
0.1442564736636067 0.0341505800317419 0.5797908568955944 T T T  
0.4019156799174352 0.9626106212611452 0.6640564696773065 T T T  
0.9040086213834549 0.5500610744111157 0.6644620015603804 T T T  
0.6451975076734099 0.4592032647702783 0.5768335191035839 T T T  
0.0712939856419369 0.6799740426521380 0.6985254721699683 T T T  
0.3537655957764953 0.4275925525007813 0.7015916439435440 T T T  
0.8392810816558790 0.0944000222212537 0.6998949069709922 T T T  
0.2802980782830568 0.9285981050857142 0.3031228796716635 T T T  
0.5627062563012741 0.1766093950920510 0.3061514417911088 T T T  
0.7713002245039891 0.5797154873837779 0.3012517185705677 T T T  
0.0343960177415582 0.3140384097074330 0.3002666523082010 T T T  
0.0048915969709473 0.6238302848352844 0.6918266575178330 T T T  
0.3638507472776236 0.2424746439013429 0.6921329306439935 T T T  
0.8647529967430135 0.2695124879792972 0.6916747052194234 T T T  
0.1083510178558528 0.5189449963030407 0.6964983898661786 T T T

0.4066061083159258	0.4688287148504545	0.7212419294298051	T	T	T
0.7716555661333356	0.1224202465101432	0.7028251678632239	T	T	T
0.2244067372976805	0.9750118047452681	0.2858691452707530	T	T	T
0.2708180765121314	0.7435445993425042	0.3122192167226145	T	T	T
0.5197373590749914	0.0267702422923335	0.3075226942589315	T	T	T
0.6264442262241295	0.1024194001079536	0.3161419705407889	T	T	T
0.7603321129236633	0.7622814735173703	0.3130039506342403	T	T	T
0.7151061615047469	0.5407157464830510	0.2836260729416541	T	T	T
0.0255155757608895	0.4961276257354311	0.3101400835771128	T	T	T
0.9759840796362551	0.2714892067837952	0.2846597924417129	T	T	T
0.6071867108102101	0.6313099236246354	0.6338992939665387	T	T	T
0.2344372928950307	0.3634625181788707	0.4844606095791164	F	F	F
0.6878585722511957	0.8797634598920726	0.3979224703726973	T	T	T

Ti O Ti O Ti O

1.0000000000000000		
14.2453041077000009	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.1680002212999998	0.0000000000000000
0.0000000000000000	0.0000000000000000	29.4789562224999990

Ti O H Co

21 56 16 3

Selective dynamics

Direct

0.0231244619920684	0.1074476182878235	0.3677518705641123	T	T	T
0.1857452070674566	0.6247485299389127	0.3964909852978356	T	T	T
0.5242214223433223	0.4012329963945737	0.3656490447003893	T	T	T
0.7675356267723831	0.3530732795258924	0.3658070419928960	T	T	T
0.9368986906274549	0.6347559319116423	0.3973748388094603	T	T	T
0.4412254845831680	0.8636901641840830	0.3996005005862962	T	T	T

0.2746539185704813	0.1521206364422850	0.3680317625954101	T	T	T
0.7342005810289152	0.1367530326270341	0.4848529224897646	F	F	F
0.3956158154875027	0.8683481241609385	0.5172283169192724	F	F	F
0.8953822014665107	0.6325289816178099	0.5172296942882255	F	F	F
0.6487817750305567	0.6455289705310605	0.5195024736345744	F	F	F
0.4815241771643173	0.3615968561732217	0.4834047030315531	F	F	F
0.1487325421792534	0.8563983739423122	0.5193773182996253	F	F	F
0.9814354254124780	0.1396032612863678	0.4834948480823442	F	F	F
0.4469479103946821	0.1363992523283520	0.6058546784972610	T	T	T
0.1059069868162898	0.8946637961518179	0.6356005576722231	T	T	T
0.9426303656791339	0.3671449631526537	0.6065361005184396	T	T	T
0.1896833833585330	0.3682245895233250	0.6053759834759818	T	T	T
0.3594647418578876	0.6539445072655941	0.6367712016337254	T	T	T
0.8535021160903755	0.8387344495540636	0.6382959741537146	T	T	T
0.6875769912449446	0.1388491477219311	0.6035267927553275	T	T	T
0.9707427969104981	0.8177032431382096	0.3416071558321561	T	T	T
0.7481441621290764	0.1739549883300259	0.4206687900153835	T	T	T
0.2531144087701876	0.3116418339578444	0.4236525475835604	T	T	T
0.4747342716844346	0.6929316430863743	0.3419442818942193	T	T	T
0.8050815347675002	0.6916732513166517	0.3964517588256042	T	T	T
0.9005155795478138	0.3178261472885484	0.3646674586132946	T	T	T
0.4104976683509338	0.1806698098666968	0.3649451886013491	T	T	T
0.3116930045654839	0.8097415354935088	0.3969219180699439	T	T	T
0.0655699246337755	0.4606634465804285	0.3903096140211242	T	T	T
0.6487548909267588	0.5483257559967410	0.3723286194412034	T	T	T
0.1483696819388527	0.9616324010394512	0.3705386891024069	T	T	T
0.5753439610687536	0.0320076153124996	0.3940145220223087	T	T	T
0.7225733467492794	0.0366708477568794	0.3393579695198002	T	T	T
0.9838318200196859	0.9642078515869973	0.4235644189337650	T	T	T

0.4869595175678708 0.5330393757963915 0.4237083157647658 T T T  
0.2310680416098299 0.4526890279643849 0.3412316152506451 T T T  
0.6690919997630900 0.8170932275262288 0.4621108699766978 F F F  
0.4563443067348629 0.1856957460417874 0.5415381954083784 F F F  
0.9563715435325619 0.3157762323396867 0.5415514049333012 F F F  
0.1684768759925106 0.6845410757490313 0.4614047933963619 F F F  
0.5163401794135183 0.6840621747006708 0.5172222351935218 F F F  
0.6122121268392959 0.3153938228045661 0.4863254931615089 F F F  
0.1121104352761861 0.1862923125396918 0.4862169103188876 F F F  
0.0164653504910319 0.8169379209085434 0.5170864510602016 F F F  
0.7737086930159478 0.4642121896258828 0.5098542901532497 F F F  
0.3547568199701061 0.5398845750144545 0.4913055491984935 F F F  
0.8548352112812623 0.9612879754852131 0.4913474116743402 F F F  
0.2736558171006749 0.0367285287095171 0.5095842622449496 F F F  
0.4364578605973435 0.0348585244096000 0.4598389770138454 F F F  
0.6931547229194095 0.9653791778681509 0.5438751113830449 F F F  
0.1930960752500894 0.5368671613790212 0.5435284188581946 F F F  
0.9363025789852344 0.4660265976351923 0.4598071447971463 F F F  
0.3754815663120877 0.8188716222140342 0.5814623846754704 T T T  
0.1551012267001035 0.1861834208711309 0.6617511635827732 T T T  
0.6525873661604996 0.3401973866982558 0.6588647194980761 T T T  
0.8753074002252519 0.6850485257082113 0.5813805833549873 T T T  
0.2263634743570600 0.6874420751683091 0.6390055109845129 T T T  
0.3212025004216034 0.3086073770069886 0.6101474233045000 T T T  
0.8172454794189651 0.1851026876434698 0.6083385201390636 T T T  
0.7182341149206375 0.8201606152221422 0.6404432133882079 T T T  
0.4858445646289421 0.4675587240387070 0.6290260310939155 T T T  
0.0617075912967293 0.5387584509430273 0.6123904582234352 T T T  
0.5630150574170888 0.9515045585111326 0.6107015210465909 T T T

0.9792617808728404	0.0324313993711267	0.6330384738194267	T	T	T
0.1453600747437425	0.0365516156854002	0.5794597199081784	T	T	T
0.4107426442484318	0.9476020151165476	0.6653359802032527	T	T	T
0.8981984175803671	0.5388784498816436	0.6636951601093369	T	T	T
0.6445326195834948	0.4719653684226145	0.5800864879989862	T	T	T
0.0919222250084304	0.6873060106711995	0.7030676972873814	T	T	T
0.3628573974541545	0.4263414518792947	0.7024878168230480	T	T	T
0.8512722771722476	0.0720559906503679	0.7019338717344464	T	T	T
0.5670381712147671	0.7663353250346576	0.6946138825894170	T	T	T
0.2797883177112148	0.9280603462174253	0.3030997252270349	T	T	T
0.5627013319499478	0.1763191001509450	0.3060271234433726	T	T	T
0.7712126679453168	0.5791492366131645	0.3011225574432587	T	T	T
0.0340650084107049	0.3134658180748419	0.3002436769577480	T	T	T
0.0986999219309404	0.5051752618814797	0.6928355117320103	T	T	T
0.3702598293773562	0.2416411058950345	0.6925596760061516	T	T	T
0.9069764355640196	0.0247379286464540	0.7192595368057668	T	T	T
0.6145480680902146	0.9012768709393952	0.6993460363856069	T	T	T
0.1515524322956693	0.7242372403562393	0.7180420973732152	T	T	T
0.4224000222601577	0.4684352008392049	0.7171228898427072	T	T	T
0.8624144725726862	0.2559090419977991	0.6918547800994505	T	T	T
0.5053988539442372	0.8612916471830295	0.6853398028652737	T	T	T
0.2234105056249202	0.9747288821035436	0.2862344698696366	T	T	T
0.2703211255188178	0.7430571454249466	0.3122763823448986	T	T	T
0.5197246876284722	0.0265883016359617	0.3074292146662668	T	T	T
0.6264322486569670	0.1020817775580506	0.3160661581111430	T	T	T
0.7603739151399240	0.7616934683524488	0.3129135103663584	T	T	T
0.7146438034707333	0.5401903319618674	0.2837771534322924	T	T	T
0.0259651033074504	0.4955781469115706	0.3102321545660013	T	T	T
0.9747791857027355	0.2721564026483013	0.2853098204258941	T	T	T



0.6060918081645083	0.6223854741885598	0.6350867580679154	T	T	T
0.2344372928950307	0.3634625181788707	0.4844606095791164	F	F	F
0.6877627865942748	0.8794513601445182	0.3977477207032516	T	T	T

=====Ni structures=====

Ti O Ti O Ti O

1.0000000000000000

14.2453041077000009 0.0000000000000000 0.0000000000000000

0.0000000000000000 5.1680002212999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 29.4789562224999990

Ti O H Ni

21 57 18 3

Selective dynamics

Direct

0.0238390023971936	0.1106550023754690	0.3674267795862945	T	T	T
0.1917659262279111	0.6390398600539975	0.3966103887674313	T	T	T
0.5234543739337578	0.3948871994379968	0.3656522836163147	T	T	T
0.7693178977168708	0.3483923282831863	0.3661582490019498	T	T	T
0.9428996511929670	0.6320536012779324	0.3969263684088145	T	T	T
0.4474957744715195	0.8677242784872665	0.3985620419802135	T	T	T
0.2746441578013243	0.1561959352218014	0.3640453371226071	T	T	T
0.7342005810289152	0.1367530326270341	0.4848529224897646	F	F	F
0.3956158154875027	0.8683481241609385	0.5172283169192724	F	F	F
0.8953822014665107	0.6325289816178099	0.5172296942882255	F	F	F
0.2344372928950307	0.3634625181788707	0.4844606095791164	F	F	F
0.4815241771643173	0.3615968561732217	0.4834047030315531	F	F	F
0.1487325421792534	0.8563983739423122	0.5193773182996253	F	F	F
0.9814354254124780	0.1396032612863678	0.4834948480823442	F	F	F
0.4446873780483472	0.1390163572930622	0.6059793141287637	T	T	T

0.1064739278977755 0.8911045867745550 0.6380289276747427 T T T  
0.9415890044369318 0.3652347070492203 0.6066455806791263 T T T  
0.1855837173660080 0.3646754867115105 0.6055387357389517 T T T  
0.3558712913319229 0.6552789418479966 0.6362806910315670 T T T  
0.8536761347084257 0.8467265748438345 0.6376913682804853 T T T  
0.6860377680393687 0.1453080736856447 0.6021337250837379 T T T  
0.6662087830943059 0.1210409750732568 0.7282813892874707 T T T  
0.9708229962524045 0.8192701908575278 0.3414757020147270 T T T  
0.7477267976218087 0.1603911448070010 0.4197676052218525 T T T  
0.2525342046412053 0.3137342415532553 0.4209699837093611 T T T  
0.4736682470529636 0.6862039765644357 0.3415173199576646 T T T  
0.8048355709175320 0.6754652836331008 0.3962041741985712 T T T  
0.9017633354471876 0.3155478435062239 0.3641877485769876 T T T  
0.4089723736609002 0.1810950716059437 0.3626943028440771 T T T  
0.3108393481092713 0.8165967308797777 0.3961222342398921 T T T  
0.0660172054800238 0.4631663735786123 0.3900820670110155 T T T  
0.6490903261488404 0.5415884636830860 0.3714840761183391 T T T  
0.1488135533549569 0.9674154215772707 0.3688941738064665 T T T  
0.5711078316727074 0.0364108244331109 0.3946656202302365 T T T  
0.7210471082457311 0.0244059089188655 0.3397750394672327 T T T  
0.9851570812861771 0.9636079427848586 0.4233352863007231 T T T  
0.4853385741046040 0.5338630439645102 0.4232198241074609 T T T  
0.2308503467656857 0.4598025780423695 0.3392692679903859 T T T  
0.6690919997630900 0.8170932275262288 0.4621108699766978 F F F  
0.4563443067348629 0.1856957460417874 0.5415381954083784 F F F  
0.9563715435325619 0.3157762323396867 0.5415514049333012 F F F  
0.1684768759925106 0.6845410757490313 0.4614047933963619 F F F  
0.5163401794135183 0.6840621747006708 0.5172222351935218 F F F  
0.6122121268392959 0.3153938228045661 0.4863254931615089 F F F

0.1121104352761861	0.1862923125396918	0.4862169103188876	F	F	F
0.0164653504910319	0.8169379209085434	0.5170864510602016	F	F	F
0.7737086930159478	0.4642121896258828	0.5098542901532497	F	F	F
0.3547568199701061	0.5398845750144545	0.4913055491984935	F	F	F
0.8548352112812623	0.9612879754852131	0.4913474116743402	F	F	F
0.2736558171006749	0.0367285287095171	0.5095842622449496	F	F	F
0.4364578605973435	0.0348585244096000	0.4598389770138454	F	F	F
0.6931547229194095	0.9653791778681509	0.5438751113830449	F	F	F
0.1930960752500894	0.5368671613790212	0.5435284188581946	F	F	F
0.9363025789852344	0.4660265976351923	0.4598071447971463	F	F	F
0.3710630029097957	0.8218406276054677	0.5809917434370592	T	T	T
0.1557245707236028	0.1861748687711295	0.6616133158714137	T	T	T
0.6575411536002402	0.3447996959973846	0.6550883938006340	T	T	T
0.8743655477215810	0.6826935190918759	0.5813177211710542	T	T	T
0.2228688116132820	0.6845664480965122	0.6411119858184009	T	T	T
0.3195767991093556	0.3142971075435338	0.6095101560609801	T	T	T
0.8191067542797421	0.1801596907738555	0.6056616965258791	T	T	T
0.7162744549697632	0.8313071349454791	0.6393638983569918	T	T	T
0.4846955618761261	0.4712678260933743	0.6274341862344440	T	T	T
0.0613150418882977	0.5350812612538997	0.6100276801538184	T	T	T
0.5608340174660804	0.9578757175713676	0.6082923645627378	T	T	T
0.9781477453743398	0.0321621155340123	0.6342345465412832	T	T	T
0.1439696051005711	0.0329667985321925	0.5797847563641855	T	T	T
0.4094921426133954	0.9491925805040641	0.6642518856893364	T	T	T
0.9017071586766137	0.5437155507987922	0.6637762424992024	T	T	T
0.6432777849295157	0.4859087283252372	0.5773949019887774	T	T	T
0.0680025882912054	0.6793575543050717	0.6988763759360082	T	T	T
0.3662193569702592	0.4331534263088189	0.7016005290854764	T	T	T
0.8469414852993322	0.0659454024901166	0.7007227577549515	T	T	T

0.5610390854667172	0.7449146797592350	0.6928141730346703	T	T	T
0.2782449043386724	0.9247700145206887	0.3008224302801789	T	T	T
0.5644115101611672	0.1812895894958079	0.3044554016678097	T	T	T
0.7705453569594547	0.5637910434205847	0.3002924132436272	T	T	T
0.0349981532639198	0.3128861635878722	0.2994653880125414	T	T	T
0.0016979401297911	0.6232317180068445	0.6919522718683850	T	T	T
0.3699355775881810	0.2466149905683897	0.6926867103455142	T	T	T
0.8657494750314512	0.2463231337581901	0.6929386441215292	T	T	T
0.6050798464408484	0.8755335330837473	0.7068422931649720	T	T	T
0.1048942537000467	0.5181471999596605	0.6971092394422883	T	T	T
0.4289203374477786	0.4737704345405638	0.7130346006649023	T	T	T
0.7829803611927106	0.0788339461971522	0.7143864236884897	T	T	T
0.5007073259075884	0.8473167182715448	0.6837995122016248	T	T	T
0.2224553188990912	0.9690277555787339	0.2833056653241902	T	T	T
0.2683654942079357	0.7400720987570020	0.3107815996809272	T	T	T
0.5193063099341027	0.0369704793055496	0.3039587839933049	T	T	T
0.6253474672294465	0.0978514713255199	0.3159714684440865	T	T	T
0.7599171179703342	0.7459051282941882	0.3120636910741894	T	T	T
0.7129558460574653	0.5233770967682817	0.2837996203901867	T	T	T
0.0293107635594945	0.4956704973318380	0.3092965130025008	T	T	T
0.9747243598285007	0.2764347381110435	0.2850609813942815	T	T	T
0.6559544212475893	0.2436556543851870	0.6999073306714040	T	T	T
0.6483155456101107	0.2166789901097370	0.7552967865455610	T	T	T
0.6038651691729048	0.6385349507684196	0.6320574852458127	T	T	T
0.6487817750305567	0.6455289705310605	0.5195024736345744	F	F	F
0.6892423125870515	0.8630478792949500	0.3968069232567035	T	T	T

Ti O Ti O Ti O

1.0000000000000000

14.2453041077000009 0.0000000000000000 0.0000000000000000  
0.0000000000000000 5.1680002212999998 0.0000000000000000  
0.0000000000000000 0.0000000000000000 29.4789562224999990

Ti O H Ni

21 57 17 3

Selective dynamics

Direct

0.0237321622326626 0.1106278325483816 0.3672769441975499 T T T  
0.1915889031940744 0.6389797467305939 0.3965593273664932 T T T  
0.5236846197940705 0.3948487439695045 0.3658393257177675 T T T  
0.7693585709581080 0.3497962064886505 0.3661592270978638 T T T  
0.9429628812994857 0.6322531972416650 0.3970480988871275 T T T  
0.4472769253784936 0.8676527899162765 0.3983980501579182 T T T  
0.2746121013514093 0.1562708509468503 0.3640234529164260 T T T  
0.7342005810289152 0.1367530326270341 0.4848529224897646 F F F  
0.3956158154875027 0.8683481241609385 0.5172283169192724 F F F  
0.8953822014665107 0.6325289816178099 0.5172296942882255 F F F  
0.2344372928950307 0.3634625181788707 0.4844606095791164 F F F  
0.4815241771643173 0.3615968561732217 0.4834047030315531 F F F  
0.1487325421792534 0.8563983739423122 0.5193773182996253 F F F  
0.9814354254124780 0.1396032612863678 0.4834948480823442 F F F  
0.4369463905255154 0.1541871744804560 0.6058079405212556 T T T  
0.1054076704298997 0.8984867561545276 0.6381431423154149 T T T  
0.9411395293675836 0.3728032998132952 0.6066679200600861 T T T  
0.1837003168387854 0.3716978257164348 0.6057010273082090 T T T  
0.3554885773844886 0.6724694640445876 0.6383073713947245 T T T  
0.8523538216173403 0.8506064590283209 0.6389951138070655 T T T  
0.6866221481845870 0.1455353622577364 0.6002398381134533 T T T  
0.6796955454836621 0.0808923546447810 0.7331073268011912 T T T

0.9708849801389863	0.8191837892505389	0.3414482683570028	T	T	T
0.7476765703006722	0.1620290061894901	0.4199140183862583	T	T	T
0.2524777848937246	0.3138818508962867	0.4209819531977299	T	T	T
0.4736973992989328	0.6861475313761680	0.3416511490467252	T	T	T
0.8048958626865106	0.6766991059958352	0.3962316928930180	T	T	T
0.9016973445475885	0.3160034288321552	0.3642676627579775	T	T	T
0.4090181765648179	0.1817124354107711	0.3627720141193414	T	T	T
0.3108614012480028	0.8166913715473840	0.3961415595417906	T	T	T
0.0660549284216132	0.4635546709687610	0.3900866659705634	T	T	T
0.6491022683165301	0.5428438687623504	0.3716922548344759	T	T	T
0.1488004222498305	0.9676271226159339	0.3688828762512179	T	T	T
0.5710940922578315	0.0375700016786345	0.3947219026545138	T	T	T
0.7210644158695714	0.0251824032691602	0.3399678236218631	T	T	T
0.9851617551290549	0.9640317889562778	0.4233024788939259	T	T	T
0.4854756055099366	0.5344551251706730	0.4233733528714110	T	T	T
0.2309856379892149	0.4600138095075830	0.3392881236424304	T	T	T
0.6690919997630900	0.8170932275262288	0.4621108699766978	F	F	F
0.4563443067348629	0.1856957460417874	0.5415381954083784	F	F	F
0.9563715435325619	0.3157762323396867	0.5415514049333012	F	F	F
0.1684768759925106	0.6845410757490313	0.4614047933963619	F	F	F
0.5163401794135183	0.6840621747006708	0.5172222351935218	F	F	F
0.6122121268392959	0.3153938228045661	0.4863254931615089	F	F	F
0.1121104352761861	0.1862923125396918	0.4862169103188876	F	F	F
0.0164653504910319	0.8169379209085434	0.5170864510602016	F	F	F
0.7737086930159478	0.4642121896258828	0.5098542901532497	F	F	F
0.3547568199701061	0.5398845750144545	0.4913055491984935	F	F	F
0.8548352112812623	0.9612879754852131	0.4913474116743402	F	F	F
0.2736558171006749	0.0367285287095171	0.5095842622449496	F	F	F
0.4364578605973435	0.0348585244096000	0.4598389770138454	F	F	F

0.6931547229194095 0.9653791778681509 0.5438751113830449 F F F  
0.1930960752500894 0.5368671613790212 0.5435284188581946 F F F  
0.9363025789852344 0.4660265976351923 0.4598071447971463 F F F  
0.3712616618111678 0.8288095385279850 0.5812125985475005 T T T  
0.1553388304984596 0.1927276033673158 0.6616035265458202 T T T  
0.6487322724162251 0.3458787424939292 0.6548428265941441 T T T  
0.8751301335102363 0.6888880677025569 0.5810723026826247 T T T  
0.2220025184536706 0.6895988943196435 0.6417985449147465 T T T  
0.3183782852475365 0.3276069616894573 0.6085620057823814 T T T  
0.8168452086032449 0.1906889958376681 0.6067529271286183 T T T  
0.7165641605627914 0.8297339107479869 0.6380903144983260 T T T  
0.4824432545482362 0.4855017749133443 0.6253585411898377 T T T  
0.0608041075610279 0.5418257133509193 0.6098645774532711 T T T  
0.5617576332616895 0.9709799116627322 0.6113822249039064 T T T  
0.9775744636805185 0.0382505836060807 0.6337097102512309 T T T  
0.1441920656824906 0.0371742587703164 0.5797863658420496 T T T  
0.4038753054174147 0.9726949937420407 0.6633534939620495 T T T  
0.9014943392352266 0.5478912619831705 0.6636018109116339 T T T  
0.6427742770930648 0.4866730413991747 0.5770411592171053 T T T  
0.0671959357564278 0.6899794426063232 0.6990270783504694 T T T  
0.3786963452779026 0.4665838559249213 0.7021780648140279 T T T  
0.8450877886854948 0.0538604547260941 0.7005086832726173 T T T  
0.5642301572217669 0.7317473376347540 0.6927011615562371 T T T  
0.2793603933661423 0.9248611276412124 0.3009820115402118 T T T  
0.5650573470862827 0.1844507038262677 0.3044605192237816 T T T  
0.7702025552832830 0.5636070932874794 0.3003612093779214 T T T  
0.0352450433104664 0.3133986322299642 0.2996014413013290 T T T  
0.0010444820254597 0.6315239248967114 0.6928150120778016 T T T  
0.3791075991442655 0.2775884479364693 0.6955584095606653 T T T

0.8651070849970177	0.2347967865662779	0.6955519226367753	T	T	T
0.6433226804463685	0.9317298350327083	0.7201868039210090	T	T	T
0.1046386558658815	0.5297853473662677	0.6984852016525942	T	T	T
0.4450514177345485	0.5117604468162215	0.7084390270130151	T	T	T
0.7782999000291347	0.0597392186352052	0.7154728521877384	T	T	T
0.5134637563238102	0.8589482153832685	0.6863507468330839	T	T	T
0.2249296895606094	0.9693932368827344	0.2825273219934664	T	T	T
0.2689193009698500	0.7401717512055818	0.3107563996858486	T	T	T
0.5196124488162218	0.0412506409763217	0.3032079217576749	T	T	T
0.6256202951300540	0.0991374512581353	0.3160300380285859	T	T	T
0.7594589614647715	0.7458820736697367	0.3119384740293953	T	T	T
0.7130328795634298	0.5225712014290760	0.2835731268437241	T	T	T
0.0283762264048314	0.4962247521730991	0.3092478175135268	T	T	T
0.9761670214323460	0.2747049553205253	0.2842646543524445	T	T	T
0.6576554054930462	0.2258156042322902	0.7140867984302129	T	T	T
0.6005003409715556	0.6434061560727720	0.6332061750995368	T	T	T
0.6487817750305567	0.6455289705310605	0.5195024736345744	F	F	F
0.6891806203243773	0.8645834540059365	0.3969123251051808	T	T	T

Ti O H Co

1.0000000000000000

14.2453041077000009 0.0000000000000000 0.0000000000000000

0.0000000000000000 5.1680002212999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 29.4789562224999990

Ti O H Ni

21 57 17 3

Selective dynamics

Direct

0.0235558140434748	0.1152737659111709	0.3682766088943645	T	T	T
--------------------	--------------------	--------------------	---	---	---



0.1886937077373054 0.6351209115390637 0.3954715438215034 T T T  
0.5256371870390570 0.3882142005598807 0.3666299361007644 T T T  
0.7676148591425452 0.3471487196250724 0.3648877801392955 T T T  
0.9371953439802234 0.6384168698998550 0.3962460329235505 T T T  
0.4465262976003713 0.8623693262262266 0.3970670395535373 T T T  
0.2752771770575541 0.1522995808368172 0.3647674879221229 T T T  
0.7342005810289152 0.1367530326270341 0.4848529224897646 F F F  
0.3956158154875027 0.8683481241609385 0.5172283169192724 F F F  
0.8953822014665107 0.6325289816178099 0.5172296942882255 F F F  
0.2344372928950307 0.3634625181788707 0.4844606095791164 F F F  
0.4815241771643173 0.3615968561732217 0.4834047030315531 F F F  
0.1487325421792534 0.8563983739423122 0.5193773182996253 F F F  
0.9814354254124780 0.1396032612863678 0.4834948480823442 F F F  
0.4478800347809388 0.1470682589151285 0.6047495285122346 T T T  
0.1053136600418371 0.9013225215799210 0.6389546627983794 T T T  
0.9400490903488253 0.3701996612708768 0.6057558158989178 T T T  
0.1817196278121717 0.3715228585635258 0.6043963330868996 T T T  
0.3527574181216742 0.6456924789041345 0.6356720039692189 T T T  
0.8529785272848666 0.8509877616592171 0.6380980624689641 T T T  
0.6865652856425407 0.1422598769537800 0.5984852838504350 T T T  
0.6118836757869486 0.9335529578886115 0.7193572265743232 T T T  
0.9700775116333565 0.8238670600140133 0.3419393079496919 T T T  
0.7461473917237639 0.1684025605675760 0.4203621665265452 T T T  
0.2523423384202416 0.3127976458669142 0.4216236119524536 T T T  
0.4727873132669939 0.6807781070987510 0.3420739979242806 T T T  
0.8055095765943300 0.6897055483281154 0.3963519013607821 T T T  
0.9015736126494812 0.3181084546213825 0.3650874665154631 T T T  
0.4085286569273112 0.1814989638347780 0.3628432771180354 T T T  
0.3105407605236490 0.8165518821923592 0.3960943594411422 T T T

0.0663889449107857 0.4653335533313144 0.3899942444253076 T T T  
0.6490191497031869 0.5456476129680237 0.3712229367193478 T T T  
0.1483314310434181 0.9668560235368829 0.3691844315400740 T T T  
0.5700119257685241 0.0391959997762453 0.3937054952449787 T T T  
0.7250477985915423 0.0504112398563341 0.3352953222520068 T T T  
0.9854255421477187 0.9667150546041051 0.4241122421405522 T T T  
0.4857072090026364 0.5324512658690013 0.4238872944935424 T T T  
0.2305795863754776 0.4579741836225089 0.3397659575882875 T T T  
0.6690919997630900 0.8170932275262288 0.4621108699766978 F F F  
0.4563443067348629 0.1856957460417874 0.5415381954083784 F F F  
0.9563715435325619 0.3157762323396867 0.5415514049333012 F F F  
0.1684768759925106 0.6845410757490313 0.4614047933963619 F F F  
0.5163401794135183 0.6840621747006708 0.5172222351935218 F F F  
0.6122121268392959 0.3153938228045661 0.4863254931615089 F F F  
0.1121104352761861 0.1862923125396918 0.4862169103188876 F F F  
0.0164653504910319 0.8169379209085434 0.5170864510602016 F F F  
0.7737086930159478 0.4642121896258828 0.5098542901532497 F F F  
0.3547568199701061 0.5398845750144545 0.4913055491984935 F F F  
0.8548352112812623 0.9612879754852131 0.4913474116743402 F F F  
0.2736558171006749 0.0367285287095171 0.5095842622449496 F F F  
0.4364578605973435 0.0348585244096000 0.4598389770138454 F F F  
0.6931547229194095 0.9653791778681509 0.5438751113830449 F F F  
0.1930960752500894 0.5368671613790212 0.5435284188581946 F F F  
0.9363025789852344 0.4660265976351923 0.4598071447971463 F F F  
0.3736627717521870 0.8283647787120908 0.5829103570000633 T T T  
0.1557461370148807 0.1936397169714150 0.6619487325230148 T T T  
0.6615163482692867 0.3428698101009304 0.6612827820452559 T T T  
0.8743756396032092 0.6876131469012446 0.5820630873294280 T T T  
0.2224980740922858 0.6908961822822375 0.6406938837156103 T T T

0.3209712059024014 0.3174713540857155 0.6100737630797459 T T T  
0.8177963114027699 0.1900779514274123 0.6059438165193207 T T T  
0.7173149199669259 0.8316351188851879 0.6406221359071155 T T T  
0.4855832467125668 0.4706399816057600 0.6317909934025403 T T T  
0.0611017538818096 0.5401656196955829 0.6099444119379388 T T T  
0.5618355219404201 0.9601824781131734 0.6119823637067134 T T T  
0.9770312788836779 0.0418930147885060 0.6360641238973200 T T T  
0.1426089309403549 0.0386694310364243 0.5804008873479910 T T T  
0.4073201214580843 0.9596158489627232 0.6672296969079370 T T T  
0.9036313338569602 0.5568635414757589 0.6648490519037427 T T T  
0.6424699532652511 0.4761705821656370 0.5803461507920417 T T T  
0.0687812047147236 0.6839778660141831 0.6988971224799444 T T T  
0.3585310040581961 0.4422636105854056 0.7026839863969772 T T T  
0.8272620734242715 0.1097542059178403 0.6987092861115158 T T T  
0.5617844875762740 0.7327017542303119 0.6967149616141579 T T T  
0.2778641479238349 0.9255633409547045 0.3010416593125467 T T T  
0.5623003176863965 0.1870743360519245 0.3034724508309431 T T T  
0.7747216805297323 0.5823317537450032 0.3011576007535002 T T T  
0.0341631023142662 0.3124038481918482 0.2997727430866631 T T T  
0.0025982703807258 0.6259373860161073 0.6912891107064790 T T T  
0.3663045037175063 0.2555197576023031 0.6945636079977499 T T T  
0.8704198016885838 0.2599159531452948 0.6949080441728490 T T T  
0.1066031453761176 0.5243107710878707 0.6971946550812852 T T T  
0.4170865518547823 0.4902724580464739 0.7177161518740343 T T T  
0.7669118234867207 0.1917656879740936 0.6899936787355584 T T T  
0.4667780401974488 0.8960476247931440 0.6820341982607846 T T T  
0.2214853134253261 0.9702606139634136 0.2840034536010485 T T T  
0.2686246356491201 0.7404863150286767 0.3107228842936852 T T T  
0.5194572985398828 0.0378215745160614 0.3034691497234514 T T T

0.6259231881481865	0.1114629406939537	0.3127241978713765	T	T	T
0.7633323549779493	0.7664021015479451	0.3118700620957239	T	T	T
0.7195750967598644	0.5405583328435697	0.2829743115358752	T	T	T
0.0281800975011681	0.4955216624776430	0.3092795639186794	T	T	T
0.9737333239801587	0.2734944123664682	0.2857057758370492	T	T	T
0.6147078308081236	0.2503283341852244	0.6796262873998210	T	T	T
0.6738263255848427	0.8547106290759413	0.7245776349666477	T	T	T
0.6048477622547448	0.6406778247738445	0.6360516055113589	T	T	T
0.6487817750305567	0.6455289705310605	0.5195024736345744	F	F	F
0.6885038197176793	0.8676224358715015	0.3970520195883612	T	T	T

Ti O H Co

1.0000000000000000

14.2453041077000009 0.0000000000000000 0.0000000000000000

0.0000000000000000 5.1680002212999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 29.4789562224999990

Ti O H Ni

21 57 16 3

Selective dynamics

Direct

0.0235726623565928	0.1149667391566420	0.3682315507428776	T	T	T
0.1886325289863213	0.6351302530391356	0.3954846286120478	T	T	T
0.5258601890150255	0.3877718430630157	0.3667204278510319	T	T	T
0.7677212876933684	0.3472714759028487	0.3649038608218657	T	T	T
0.9372604970457291	0.6382458426189919	0.3963041796929066	T	T	T
0.4464451163588893	0.8619847466967293	0.3969410374758852	T	T	T
0.2753352460075164	0.1524741441849350	0.3647587176791790	T	T	T
0.7342005810289152	0.1367530326270341	0.4848529224897646	F	F	F
0.3956158154875027	0.8683481241609385	0.5172283169192724	F	F	F

0.8953822014665107 0.6325289816178099 0.5172296942882255 F F F  
0.2344372928950307 0.3634625181788707 0.4844606095791164 F F F  
0.4815241771643173 0.3615968561732217 0.4834047030315531 F F F  
0.1487325421792534 0.8563983739423122 0.5193773182996253 F F F  
0.9814354254124780 0.1396032612863678 0.4834948480823442 F F F  
0.4488525728200929 0.1499608633309178 0.6045630264317425 T T T  
0.1054912652732867 0.9013101009623190 0.6388348229388530 T T T  
0.9400346757501447 0.3697251029238177 0.6055977781408440 T T T  
0.1813558975411483 0.3723049260811390 0.6043001008761076 T T T  
0.3530643177816661 0.6444304170276871 0.6355548779769851 T T T  
0.8535175132707550 0.8496092885053192 0.6386474994366308 T T T  
0.6875425754924670 0.1419586465727140 0.5986153175383510 T T T  
0.5736772286580075 0.9514101171953303 0.7157672984892113 T T T  
0.9702108729066963 0.8235281965524055 0.3419354369339603 T T T  
0.7461813694649891 0.1684790329313651 0.4203464627602461 T T T  
0.2524743725550927 0.3128781502722150 0.4216446496924989 T T T  
0.4728092775094889 0.6804053276015009 0.3421029175984406 T T T  
0.8056071689469848 0.6898281789876839 0.3963298670418363 T T T  
0.9016629739987896 0.3180783251124956 0.3650985544077793 T T T  
0.4086197154862847 0.1815015896998984 0.3628453551584810 T T T  
0.3106194173280075 0.8164921783213360 0.3961081665496090 T T T  
0.0665118775688208 0.4652172845832967 0.3899897666477204 T T T  
0.6490799464710613 0.5457292753557196 0.3712653869064588 T T T  
0.1484577417695575 0.9668965782005453 0.3691784092555013 T T T  
0.5700431403070573 0.0393408720896396 0.3936966944883526 T T T  
0.7251041885803972 0.0502723778952255 0.3353536517167255 T T T  
0.9855004608635857 0.9666544841295265 0.4241013958889789 T T T  
0.4857075399293002 0.5323482223423128 0.4239385748249426 T T T  
0.2307045103009733 0.4580145433098171 0.3397654285081159 T T T

0.6690919997630900 0.8170932275262288 0.4621108699766978 F F F  
0.4563443067348629 0.1856957460417874 0.5415381954083784 F F F  
0.9563715435325619 0.3157762323396867 0.5415514049333012 F F F  
0.1684768759925106 0.6845410757490313 0.4614047933963619 F F F  
0.5163401794135183 0.6840621747006708 0.5172222351935218 F F F  
0.6122121268392959 0.3153938228045661 0.4863254931615089 F F F  
0.1121104352761861 0.1862923125396918 0.4862169103188876 F F F  
0.0164653504910319 0.8169379209085434 0.5170864510602016 F F F  
0.7737086930159478 0.4642121896258828 0.5098542901532497 F F F  
0.3547568199701061 0.5398845750144545 0.4913055491984935 F F F  
0.8548352112812623 0.9612879754852131 0.4913474116743402 F F F  
0.2736558171006749 0.0367285287095171 0.5095842622449496 F F F  
0.4364578605973435 0.0348585244096000 0.4598389770138454 F F F  
0.6931547229194095 0.9653791778681509 0.5438751113830449 F F F  
0.1930960752500894 0.5368671613790212 0.5435284188581946 F F F  
0.9363025789852344 0.4660265976351923 0.4598071447971463 F F F  
0.3751129401612281 0.8312818149597779 0.5834058406565068 T T T  
0.1567090844686659 0.1931810608752825 0.6618026812452845 T T T  
0.6604821379028161 0.3386750825497041 0.6611269614010900 T T T  
0.8748788409778331 0.6874929684809711 0.5820760649583060 T T T  
0.2225575807045994 0.6909726152008053 0.6402170091237964 T T T  
0.3214592669396654 0.3217406843596262 0.6090761787126866 T T T  
0.8180264494464002 0.1896294494446055 0.6058898429453685 T T T  
0.7181109252901130 0.8317522124253076 0.6404072296931085 T T T  
0.4848183665619921 0.4711636645156964 0.6338186906324585 T T T  
0.0611733603336010 0.5401275926060892 0.6099052401146627 T T T  
0.5609928480799317 0.9608794342812227 0.6139653038004766 T T T  
0.9776316528793798 0.0404119010105806 0.6355583088163215 T T T  
0.1427381503636877 0.0389019868513907 0.5802370220228673 T T T

0.3997017266047887	0.9718260701085458	0.6677701529760008	T	T	T
0.9032394267022511	0.5524945601964073	0.6647188765169405	T	T	T
0.6411236325339126	0.4736830358908821	0.5799951813273980	T	T	T
0.0693112332637036	0.6837290684817530	0.6988233432196003	T	T	T
0.3487578399092115	0.4443912551544226	0.7027802321258618	T	T	T
0.8354025269634798	0.0995031281862110	0.6991298460385105	T	T	T
0.5786506795121737	0.7172706822517889	0.7011230860820529	T	T	T
0.2782164459658557	0.9255926182624775	0.3010635089305054	T	T	T
0.5626060750544045	0.1879507586762205	0.3034569429246443	T	T	T
0.7747298674838594	0.5821583327904997	0.3011459399182929	T	T	T
0.0341872946156049	0.3124104887318194	0.2997837282888730	T	T	T
0.0030550131684399	0.6256572401745361	0.6918403028020641	T	T	T
0.3522965063679255	0.2580262511274207	0.6935120238830643	T	T	T
0.8668551817589568	0.2682438662453024	0.6919434064841975	T	T	T
0.1069559002395035	0.5237868143442460	0.6971231628583680	T	T	T
0.4059327827430121	0.4754896681635941	0.7200825962190257	T	T	T
0.7687076535937339	0.1473369563838917	0.6985238604310274	T	T	T
0.4542036229390972	0.9570837978580919	0.6877121864144961	T	T	T
0.2220053740637826	0.9700930430493999	0.2838835738046790	T	T	T
0.2689529069690735	0.7405395428152278	0.3107402071128227	T	T	T
0.5196016071938607	0.0391163016321995	0.3032416236044086	T	T	T
0.6261008084339862	0.1117097519096049	0.3127526598129688	T	T	T
0.7633702494176008	0.7662388513476104	0.3118647819445147	T	T	T
0.7195582888927071	0.5404252897585751	0.2829694671042385	T	T	T
0.0281405000611506	0.4954791753742150	0.3092873630416229	T	T	T
0.9738672576088426	0.2734440473670920	0.2856239076724694	T	T	T
0.6101963973797188	0.2393190495003115	0.6760755295681643	T	T	T
0.6058154513953630	0.6390673579512545	0.6365526715715631	T	T	T
0.6487817750305567	0.6455289705310605	0.5195024736345744	F	F	F

0.6885611900143944 0.8678064871777458 0.3970502491173500 T T T

Ti O H Co

1.0000000000000000

14.2453041077000009 0.0000000000000000 0.0000000000000000

0.0000000000000000 5.1680002212999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 29.4789562224999990

Ti O H Ni

21 57 15 3

Selective dynamics

Direct

0.0237223572051023 0.1117016313223213 0.3674252618968392 T T T

0.1915102997992464 0.6393008340173355 0.3965868135215559 T T T

0.5234075305186336 0.3959017095152385 0.3657065810123392 T T T

0.7690301291792829 0.3508416084603734 0.3661920136183406 T T T

0.9425489676669342 0.6331821662091190 0.3969168310442741 T T T

0.4472417206480148 0.8684261898294092 0.3985356721676449 T T T

0.2745268343227453 0.1566643765415685 0.3640155670637233 T T T

0.7342005810289152 0.1367530326270341 0.4848529224897646 F F F

0.3956158154875027 0.8683481241609385 0.5172283169192724 F F F

0.8953822014665107 0.6325289816178099 0.5172296942882255 F F F

0.2344372928950307 0.3634625181788707 0.4844606095791164 F F F

0.4815241771643173 0.3615968561732217 0.4834047030315531 F F F

0.1487325421792534 0.8563983739423122 0.5193773182996253 F F F

0.9814354254124780 0.1396032612863678 0.4834948480823442 F F F

0.4411455635555927 0.1477710891829142 0.6065544497681136 T T T

0.1075078086498494 0.8968381473491053 0.6377112602234977 T T T

0.9426824830606633 0.3730180175613264 0.6066370349960397 T T T

0.1868606581061527 0.3708817045887213 0.6054273101240196 T T T



0.3582659666517744	0.6671351915316984	0.6379519544326300	T	T	T
0.8530554671412550	0.8555577923937655	0.6371477062226705	T	T	T
0.6860286168292221	0.1472211767612489	0.5989571860369051	T	T	T
0.5941916224928622	0.9431229221339840	0.7163897450347240	T	T	T
0.9706446897146604	0.8201201879223450	0.3415092747075025	T	T	T
0.7473797318174709	0.1632266846805933	0.4200251307514526	T	T	T
0.2524303362478881	0.3142634763233978	0.4209555767813715	T	T	T
0.4736372665994499	0.6872288565727948	0.3415397304117037	T	T	T
0.8047805069043741	0.6779119000708478	0.3963496936278094	T	T	T
0.9014413634503128	0.3166803422608591	0.3643256538846267	T	T	T
0.4088323895874982	0.1821338140108411	0.3627458550268048	T	T	T
0.3107268432276394	0.8170433293567722	0.3960886874518446	T	T	T
0.0658648227295466	0.4639639218414078	0.3900588127913751	T	T	T
0.6489466136327812	0.5438975969160772	0.3716299051825440	T	T	T
0.1485822049981250	0.9680534110937330	0.3689045121579113	T	T	T
0.5709179952692660	0.0382983504865251	0.3946861944230818	T	T	T
0.7211107156291876	0.0270710140615306	0.3398884976742538	T	T	T
0.9850606567730484	0.9644750658659418	0.4233653226922332	T	T	T
0.4853759346477370	0.5348654382443668	0.4232698139990596	T	T	T
0.2306594596609901	0.4602554105102467	0.3392606044681628	T	T	T
0.6690919997630900	0.8170932275262288	0.4621108699766978	F	F	F
0.4563443067348629	0.1856957460417874	0.5415381954083784	F	F	F
0.9563715435325619	0.3157762323396867	0.5415514049333012	F	F	F
0.1684768759925106	0.6845410757490313	0.4614047933963619	F	F	F
0.5163401794135183	0.6840621747006708	0.5172222351935218	F	F	F
0.6122121268392959	0.3153938228045661	0.4863254931615089	F	F	F
0.1121104352761861	0.1862923125396918	0.4862169103188876	F	F	F
0.0164653504910319	0.8169379209085434	0.5170864510602016	F	F	F
0.7737086930159478	0.4642121896258828	0.5098542901532497	F	F	F

0.3547568199701061 0.5398845750144545 0.4913055491984935 F F F  
0.8548352112812623 0.9612879754852131 0.4913474116743402 F F F  
0.2736558171006749 0.0367285287095171 0.5095842622449496 F F F  
0.4364578605973435 0.0348585244096000 0.4598389770138454 F F F  
0.6931547229194095 0.9653791778681509 0.5438751113830449 F F F  
0.1930960752500894 0.5368671613790212 0.5435284188581946 F F F  
0.9363025789852344 0.4660265976351923 0.4598071447971463 F F F  
0.3745050797116196 0.8215275420292022 0.5811738477175452 T T T  
0.1561554885243789 0.1914817223345179 0.6613637647481995 T T T  
0.6575451348614342 0.3520139996541922 0.6595056653354391 T T T  
0.8740827820007071 0.6903228237550515 0.5810254453233253 T T T  
0.2223287752362724 0.6889399163242539 0.6404033761838611 T T T  
0.3192716516856179 0.3221067564973216 0.6077393759413140 T T T  
0.8164853096120858 0.1932312474973265 0.6054953607054054 T T T  
0.7161786057438325 0.8398858353952048 0.6394614679621849 T T T  
0.4843643049338106 0.4772011876551901 0.6311556355156985 T T T  
0.0603202157406187 0.5412913769638037 0.6098186747385567 T T T  
0.5615011223133910 0.9715470199643861 0.6118184803271746 T T T  
0.9767352753092695 0.0415991245583662 0.6346882196284634 T T T  
0.1432627208011367 0.0370977808861464 0.5794631466217521 T T T  
0.4003217185733157 0.9689326070458156 0.6634702615173883 T T T  
0.9011209655769176 0.5551904624338516 0.6638272886828175 T T T  
0.6423783363377935 0.4865172788353334 0.5777735172720653 T T T  
0.0680554345482892 0.6875826180451423 0.6987091357454290 T T T  
0.3545163506402434 0.4362959156517690 0.7016211481077873 T T T  
0.8354721375903353 0.0967625441794723 0.6989642918005926 T T T  
0.5673843848866751 0.7354751568869540 0.6980099873668778 T T T  
0.2782535896678643 0.9255526574744076 0.3008740751375338 T T T  
0.5642002465662336 0.1829575707603090 0.3044388631602992 T T T

0.7706969754879832	0.5673322170660341	0.3005791903656546	T	T	T
0.0344904787320612	0.3137061790867057	0.2995349872638628	T	T	T
0.0018341422045586	0.6309522525417216	0.6918511611579763	T	T	T
0.3637975263611291	0.2507690496740094	0.6923742068723460	T	T	T
0.8620111528878986	0.2710741632024786	0.6912554530911191	T	T	T
0.1051710939108872	0.5267470322429058	0.6974989182307365	T	T	T
0.4090809160575734	0.4802028856526871	0.7200093196875842	T	T	T
0.7678310463933051	0.1289168694748753	0.7008953039951699	T	T	T
0.2228052384815415	0.9700270995472233	0.2831289020858458	T	T	T
0.2682296058700560	0.7408471045484175	0.3107598066700074	T	T	T
0.5191323204794975	0.0385560262118456	0.3038898779526210	T	T	T
0.6251563695606983	0.0996792694578948	0.3158890146422415	T	T	T
0.7597771496642761	0.7494970750391221	0.3122986542723320	T	T	T
0.7135892270872884	0.5267321402729132	0.2837265181820222	T	T	T
0.0283160903981677	0.4965016275152346	0.3093023836755318	T	T	T
0.9745489063220047	0.2760785101703886	0.2849059040774145	T	T	T
0.6061391207777610	0.2564148159891926	0.6740691052291322	T	T	T
0.6032993188727352	0.6518431318016434	0.6339129757621422	T	T	T
0.6487817750305567	0.6455289705310605	0.5195024736345744	F	F	F
0.6889411062037251	0.8657079788622611	0.3969599190836065	T	T	T

Ti O H Co

1.000000000000000		
14.2453041077000009	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.1680002212999998	0.0000000000000000
0.0000000000000000	0.0000000000000000	29.4789562224999990

Ti O H Ni

21 55 15 3

Selective dynamics

## Direct

0.0239104899910225	0.1132521591684309	0.3677231042076952	T	T	T
0.1909969052342241	0.6387369900338710	0.3963651580558621	T	T	T
0.5241730554510620	0.3948867573289184	0.3660366598343242	T	T	T
0.7686988334591908	0.3511523352788666	0.3659795541009819	T	T	T
0.9413442695585924	0.6349955111527967	0.3966686719695121	T	T	T
0.4472142053742334	0.8676396795859931	0.3982035817729692	T	T	T
0.2749307561487754	0.1561605471018722	0.3642189591619415	T	T	T
0.7342005810289152	0.1367530326270341	0.4848529224897646	F	F	F
0.3956158154875027	0.8683481241609385	0.5172283169192724	F	F	F
0.8953822014665107	0.6325289816178099	0.5172296942882255	F	F	F
0.2344372928950307	0.3634625181788707	0.4844606095791164	F	F	F
0.4815241771643173	0.3615968561732217	0.4834047030315531	F	F	F
0.1487325421792534	0.8563983739423122	0.5193773182996253	F	F	F
0.9814354254124780	0.1396032612863678	0.4834948480823442	F	F	F
0.4399064611897565	0.1498396966042266	0.6062182434726455	T	T	T
0.1075860609830719	0.8988185564086690	0.6378358057631024	T	T	T
0.9426338593010548	0.3735157824975365	0.6065114101964384	T	T	T
0.1863114123616930	0.3729948870594785	0.6053094223663822	T	T	T
0.3586699895355819	0.6691312223434672	0.6384905967758014	T	T	T
0.8528893219354827	0.8554154298123349	0.6374010431889469	T	T	T
0.6863973425830902	0.1425844130424275	0.5990920094173129	T	T	T
0.9705857333563238	0.8214963507185969	0.3416521941932064	T	T	T
0.7473234824936248	0.1658054787340977	0.4202140745551028	T	T	T
0.2525116758030040	0.3140362089050365	0.4211278795580825	T	T	T
0.4735278635346008	0.6862082162676928	0.3417362822029297	T	T	T
0.8050441225859888	0.6809389142672133	0.3964472509943963	T	T	T
0.9014387395423223	0.3174905436306983	0.3644584564092961	T	T	T
0.4089099857039588	0.1826973397750615	0.3628035988504295	T	T	T

0.3107590703928364 0.8173020893166558 0.3960759146033251 T T T  
0.0660408496087467 0.4645701252284090 0.3900074392716694 T T T  
0.6490275224923931 0.5456457027992727 0.3717456783807795 T T T  
0.1486084709521129 0.9681093358484667 0.3690478830502488 T T T  
0.5707212782927232 0.0398637726624906 0.3944937226180285 T T T  
0.7218422131814440 0.0324436463013620 0.3392907319652720 T T T  
0.9852471286631389 0.9652615942245506 0.4235454003198214 T T T  
0.4854362947681163 0.5349331692331984 0.4234828155369845 T T T  
0.2307565555115111 0.4601566939243683 0.3394100397367666 T T T  
0.6690919997630900 0.8170932275262288 0.4621108699766978 F F F  
0.4563443067348629 0.1856957460417874 0.5415381954083784 F F F  
0.9563715435325619 0.3157762323396867 0.5415514049333012 F F F  
0.1684768759925106 0.6845410757490313 0.4614047933963619 F F F  
0.5163401794135183 0.6840621747006708 0.5172222351935218 F F F  
0.6122121268392959 0.3153938228045661 0.4863254931615089 F F F  
0.1121104352761861 0.1862923125396918 0.4862169103188876 F F F  
0.0164653504910319 0.8169379209085434 0.5170864510602016 F F F  
0.7737086930159478 0.4642121896258828 0.5098542901532497 F F F  
0.3547568199701061 0.5398845750144545 0.4913055491984935 F F F  
0.8548352112812623 0.9612879754852131 0.4913474116743402 F F F  
0.2736558171006749 0.0367285287095171 0.5095842622449496 F F F  
0.4364578605973435 0.0348585244096000 0.4598389770138454 F F F  
0.6931547229194095 0.9653791778681509 0.5438751113830449 F F F  
0.1930960752500894 0.5368671613790212 0.5435284188581946 F F F  
0.9363025789852344 0.4660265976351923 0.4598071447971463 F F F  
0.3749864773901798 0.8230589549429784 0.5817038223238161 T T T  
0.1558562826168294 0.1936861534745947 0.6614758366665046 T T T  
0.6522843802605537 0.3530301309868023 0.6606921015056716 T T T  
0.8737919540899411 0.6909797261493540 0.5813129611581086 T T T

0.2225689484516575 0.6908244513756783 0.6403207519868979 T T T  
0.3193969997955978 0.3224775723717952 0.6080180847726283 T T T  
0.8160009382522755 0.1949947952427811 0.6060278606124655 T T T  
0.7154035636060645 0.8358726583483984 0.6399277991362576 T T T  
0.4848981906210393 0.4791021617539357 0.6320510009674585 T T T  
0.0603624798166734 0.5424155819308129 0.6098125600178251 T T T  
0.5610676570683940 0.9714829190657620 0.6130072349613565 T T T  
0.9764173214612611 0.0429624066199739 0.6350093075855548 T T T  
0.1431865587604716 0.0386405039842617 0.5796161829697319 T T T  
0.4013999726741007 0.9685274648902171 0.6644163503393506 T T T  
0.9018221157258429 0.5569234899787370 0.6641155575905497 T T T  
0.6427194911633214 0.4800901396162369 0.5768938635387940 T T T  
0.0686374865687705 0.6872493396297696 0.6986631452754609 T T T  
0.3510889074011412 0.4300205712580190 0.7012460638556154 T T T  
0.8314488547106691 0.1033669494285623 0.6986364993605595 T T T  
0.2780619497253021 0.9261514165299271 0.3009052781749504 T T T  
0.5642122121505112 0.1850737180865004 0.3042262931236601 T T T  
0.7710325074399128 0.5718296283028689 0.3007631084740870 T T T  
0.0343653617487911 0.3132184363579452 0.2995494859309759 T T T  
0.0023067522391456 0.6312756789270674 0.6917085936567764 T T T  
0.3629094639291852 0.2452140898002817 0.6917741317800163 T T T  
0.8624988298510894 0.2726415368805120 0.6915039112835328 T T T  
0.1055978905633775 0.5261380767675302 0.6969635392947124 T T T  
0.4004905780885814 0.4733034759306053 0.7227178744949767 T T T  
0.7645744522961596 0.1483889026056314 0.6973794740320085 T T T  
0.2221136541897911 0.9705704599254812 0.2835245008756440 T T T  
0.2684316470716033 0.7412298385140522 0.3107222578625783 T T T  
0.5194911366359098 0.0399483282965304 0.3037270379976922 T T T  
0.6255779881865270 0.1029232624828036 0.3153899387583628 T T T

0.7600441922327311	0.7541847220408940	0.3124369419971769	T	T	T
0.7140438457766299	0.5311480342712839	0.2838327330877216	T	T	T
0.0287513307993324	0.4961845870968208	0.3092266044909643	T	T	T
0.9739932640562498	0.2761016045840078	0.2852936203803429	T	T	T
0.5949951746573073	0.2612247596322638	0.6697709662546488	T	T	T
0.6035976688005770	0.6484699448306384	0.6311191130948040	T	T	T
0.6487817750305567	0.6455289705310605	0.5195024736345744	F	F	F
0.6889461065950937	0.8681391338413844	0.3971541759333335	T	T	T

Ti O H Co

1.0000000000000000		
14.2453041077000009	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.1680002212999998	0.0000000000000000
0.0000000000000000	0.0000000000000000	29.4789562224999990

Ti O H Ni

21 55 14 3

Selective dynamics

Direct

0.0237476481054750	0.1127477856152023	0.3676300980535634	T	T	T
0.1912161713523172	0.6390181503202196	0.3964413954607328	T	T	T
0.5237749972510887	0.3953581509067201	0.3658734865497234	T	T	T
0.7687522163518239	0.3508866511220823	0.3660382192131082	T	T	T
0.9417872531998815	0.6342887938938092	0.3967359150330228	T	T	T
0.4472509242265524	0.8679927112519057	0.3983382083921729	T	T	T
0.2746976474759675	0.1562547481960214	0.3641496091074920	T	T	T
0.7342005810289152	0.1367530326270341	0.4848529224897646	F	F	F
0.3956158154875027	0.8683481241609385	0.5172283169192724	F	F	F
0.8953822014665107	0.6325289816178099	0.5172296942882255	F	F	F
0.2344372928950307	0.3634625181788707	0.4844606095791164	F	F	F

0.4815241771643173 0.3615968561732217 0.4834047030315531 F F F  
0.1487325421792534 0.8563983739423122 0.5193773182996253 F F F  
0.9814354254124780 0.1396032612863678 0.4834948480823442 F F F  
0.4385794053477404 0.1515070432242444 0.6064347448608157 T T T  
0.1075827308385862 0.8967417525366463 0.6380280091909247 T T T  
0.9421728843069557 0.3696988034406426 0.6066208456812858 T T T  
0.1852525864010847 0.3718059538448906 0.6053043032840694 T T T  
0.3583624316817943 0.6687836402813547 0.6382797449995695 T T T  
0.8531204040091711 0.8517186744579794 0.6373379243659542 T T T  
0.6853719368971080 0.1429519591104515 0.6006985176951486 T T T  
0.9704810489523987 0.8210608278829844 0.3416135364478721 T T T  
0.7473865407261923 0.1643953479993035 0.4200158917869767 T T T  
0.2524312065539581 0.3140779919412253 0.4210668622482614 T T T  
0.4734363826870541 0.6865920433693578 0.3416366618450311 T T T  
0.8048165080835599 0.6793294648439744 0.3963937124868225 T T T  
0.9014210672470321 0.3171997266112503 0.3643556796453639 T T T  
0.4087654234051452 0.1824166493359206 0.3627771437824394 T T T  
0.3106714931069977 0.8171290813482422 0.3960929301064748 T T T  
0.0658874617850320 0.4643072124704938 0.3900297327551928 T T T  
0.6489248718236728 0.5446420765637147 0.3716322287355681 T T T  
0.1485053067452794 0.9680447601272526 0.3689978817282944 T T T  
0.5707230238940236 0.0391247882218319 0.3945567847197454 T T T  
0.7213534863570610 0.0294925018346997 0.3395810249377149 T T T  
0.9851072779984046 0.9648774036117367 0.4234870354883509 T T T  
0.4853906735321848 0.5349604223880964 0.4233835909338929 T T T  
0.2306210063441320 0.4600811835898958 0.3393571778709802 T T T  
0.6690919997630900 0.8170932275262288 0.4621108699766978 F F F  
0.4563443067348629 0.1856957460417874 0.5415381954083784 F F F  
0.9563715435325619 0.3157762323396867 0.5415514049333012 F F F



0.1684768759925106	0.6845410757490313	0.4614047933963619	F	F	F
0.5163401794135183	0.6840621747006708	0.5172222351935218	F	F	F
0.6122121268392959	0.3153938228045661	0.4863254931615089	F	F	F
0.1121104352761861	0.1862923125396918	0.4862169103188876	F	F	F
0.0164653504910319	0.8169379209085434	0.5170864510602016	F	F	F
0.7737086930159478	0.4642121896258828	0.5098542901532497	F	F	F
0.3547568199701061	0.5398845750144545	0.4913055491984935	F	F	F
0.8548352112812623	0.9612879754852131	0.4913474116743402	F	F	F
0.2736558171006749	0.0367285287095171	0.5095842622449496	F	F	F
0.4364578605973435	0.0348585244096000	0.4598389770138454	F	F	F
0.6931547229194095	0.9653791778681509	0.5438751113830449	F	F	F
0.1930960752500894	0.5368671613790212	0.5435284188581946	F	F	F
0.9363025789852344	0.4660265976351923	0.4598071447971463	F	F	F
0.3741144936496040	0.8232565164132465	0.5814166623669743	T	T	T
0.1560487861408535	0.1917633804959927	0.6615436348223946	T	T	T
0.6528827238239605	0.3590993392415144	0.6555297437922737	T	T	T
0.8737728855127145	0.6882968396156867	0.5812981456104174	T	T	T
0.2222812795260464	0.6885423738434507	0.6404762165800990	T	T	T
0.3187878995153032	0.3211970029867545	0.6078143830242572	T	T	T
0.8166443652496559	0.1907356025081002	0.6060681669551443	T	T	T
0.7162327599057087	0.8348776294957160	0.6405735029722478	T	T	T
0.4831986937769007	0.4797579425692106	0.6304090778943354	T	T	T
0.0602194152395812	0.5404162857325020	0.6098528784915451	T	T	T
0.5616621891973388	0.9655153638837076	0.6128463723033964	T	T	T
0.9768223220646916	0.0397850452196232	0.6350040277516357	T	T	T
0.1430225656467958	0.0371245435152584	0.5796705959493150	T	T	T
0.4011456616922470	0.9684306409733352	0.6639320179234701	T	T	T
0.9012546583352443	0.5515060298351223	0.6640904598180556	T	T	T
0.6425246568003099	0.4778418459542870	0.5753410290169934	T	T	T

0.0683425881711725	0.6845646540431851	0.6987072372930259	T	T	T
0.3549194944619798	0.4338758921554112	0.7014772076091883	T	T	T
0.8347653910724133	0.0943543104578231	0.6993572643468429	T	T	T
0.2779865299517161	0.9259135832962214	0.3008870773171223	T	T	T
0.5640750465506118	0.1840052607355876	0.3042960188824904	T	T	T
0.7709313116848350	0.5697633531988953	0.3006035160569627	T	T	T
0.0345884473642049	0.3129727176652269	0.2995189716014643	T	T	T
0.0021188178588991	0.6278075055682185	0.6918173004733053	T	T	T
0.3644180483067045	0.2483691430822062	0.6920502875504702	T	T	T
0.8604299635293625	0.2694705273867266	0.6913808364298903	T	T	T
0.1055021205273070	0.5237501394079560	0.6971581656908555	T	T	T
0.4089452426346566	0.4754509944433153	0.7203527888113734	T	T	T
0.7670202091590745	0.1222633187956294	0.7017316096571203	T	T	T
0.2222011585829217	0.9704479897372520	0.2833921394417790	T	T	T
0.2682192144619437	0.7410815946456439	0.3107177886673677	T	T	T
0.5191403550705543	0.0393200986581344	0.3037677814510408	T	T	T
0.6252084766505905	0.1012286594404217	0.3155979619365322	T	T	T
0.7599471755719300	0.7519450218702344	0.3123388418530845	T	T	T
0.7139446116145913	0.5294278398396198	0.2836392050783623	T	T	T
0.0290066884619464	0.4959275252055764	0.3092124854605202	T	T	T
0.9743183030055966	0.2762447115635821	0.2851306223159736	T	T	T
0.6036289603349149	0.6403904754736379	0.6313303316171697	T	T	T
0.6487817750305567	0.6455289705310605	0.5195024736345744	F	F	F
0.6888859060042826	0.8670734000151690	0.3970575162585384	T	T	T

Ti O Ti O Ti O

1.0000000000000000

14.2453041077000009 0.0000000000000000 0.0000000000000000

0.0000000000000000 5.1680002212999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 29.4789562224999990

Ti O H Ni

21 56 16 3

Selective dynamics

Direct

0.0237063581810422	0.1105735231798923	0.3674362336624534	T	T	T
0.1916345439946014	0.6387805017075131	0.3965692371029628	T	T	T
0.5233740893673478	0.3943773822871958	0.3656689276840441	T	T	T
0.7691630915524523	0.3474962426633074	0.3661038231589769	T	T	T
0.9427012817296431	0.6319347515949707	0.3968924248746173	T	T	T
0.4474640341970620	0.8673892093328123	0.3985276591844292	T	T	T
0.2745354992356852	0.1558727916127363	0.3640626527932300	T	T	T
0.7342005810289152	0.1367530326270341	0.4848529224897646	F	F	F
0.3956158154875027	0.8683481241609385	0.5172283169192724	F	F	F
0.8953822014665107	0.6325289816178099	0.5172296942882255	F	F	F
0.2344372928950307	0.3634625181788707	0.4844606095791164	F	F	F
0.4815241771643173	0.3615968561732217	0.4834047030315531	F	F	F
0.1487325421792534	0.8563983739423122	0.5193773182996253	F	F	F
0.9814354254124780	0.1396032612863678	0.4834948480823442	F	F	F
0.4456413835140800	0.1373470683962492	0.6057070215315404	T	T	T
0.1037890880773340	0.8902045992866119	0.6350112623326574	T	T	T
0.9386519417145216	0.3632607351713381	0.6070102748383083	T	T	T
0.1870462239583454	0.3673596486442032	0.6069232061022961	T	T	T
0.3576183696708271	0.6547512786793913	0.6361987591324958	T	T	T
0.8517013320165100	0.8402133252177777	0.6373749182492854	T	T	T
0.6844636383189703	0.1472548376908056	0.6033813194848475	T	T	T
0.9706769652332262	0.8190267805161917	0.3414774032620164	T	T	T
0.7476357708440670	0.1594682634544748	0.4196483262178923	T	T	T
0.2524425926351647	0.3136522617917946	0.4209646827114973	T	T	T

0.4735572948066294	0.6856939075491350	0.3415124032340143	T	T	T
0.8047057249825611	0.6749317818267381	0.3961357321835196	T	T	T
0.9016867826718377	0.3153532154328511	0.3641584389702532	T	T	T
0.4088174825929080	0.1806568749119370	0.3626843238446093	T	T	T
0.3107131066390142	0.8162915341932150	0.3961383789862736	T	T	T
0.0658750911679215	0.4629564874141537	0.3900577751961721	T	T	T
0.6489770856096461	0.5407686719664359	0.3714349534460529	T	T	T
0.1486578548091674	0.9672085068663854	0.3688603365294204	T	T	T
0.5709987240499906	0.0358418505008826	0.3946409335875904	T	T	T
0.7208996797864434	0.0236917881393050	0.3396675045883947	T	T	T
0.9851052591119781	0.9634547080596580	0.4233486517571836	T	T	T
0.4853526307028249	0.5336400973386615	0.4232250304749990	T	T	T
0.2307555099389379	0.4595100359892661	0.3392522589250847	T	T	T
0.6690919997630900	0.8170932275262288	0.4621108699766978	F	F	F
0.4563443067348629	0.1856957460417874	0.5415381954083784	F	F	F
0.9563715435325619	0.3157762323396867	0.5415514049333012	F	F	F
0.1684768759925106	0.6845410757490313	0.4614047933963619	F	F	F
0.5163401794135183	0.6840621747006708	0.5172222351935218	F	F	F
0.6122121268392959	0.3153938228045661	0.4863254931615089	F	F	F
0.1121104352761861	0.1862923125396918	0.4862169103188876	F	F	F
0.0164653504910319	0.8169379209085434	0.5170864510602016	F	F	F
0.7737086930159478	0.4642121896258828	0.5098542901532497	F	F	F
0.3547568199701061	0.5398845750144545	0.4913055491984935	F	F	F
0.8548352112812623	0.9612879754852131	0.4913474116743402	F	F	F
0.2736558171006749	0.0367285287095171	0.5095842622449496	F	F	F
0.4364578605973435	0.0348585244096000	0.4598389770138454	F	F	F
0.6931547229194095	0.9653791778681509	0.5438751113830449	F	F	F
0.1930960752500894	0.5368671613790212	0.5435284188581946	F	F	F
0.9363025789852344	0.4660265976351923	0.4598071447971463	F	F	F

0.3720376222428594 0.8208794003451380 0.5810336804094220 T T T  
0.1541750843718193 0.1835758328657065 0.6616693372099762 T T T  
0.6543947080648722 0.3368829688546099 0.6555654916050919 T T T  
0.8749311402211217 0.6837694322975286 0.5810453979956623 T T T  
0.2247342744621321 0.6883322371816769 0.6397714879253669 T T T  
0.3196429122015418 0.3112792078193369 0.6101871914218058 T T T  
0.8185713816408565 0.1801898790390317 0.6062757844448905 T T T  
0.7159566396058976 0.8246950839728664 0.6386768638220274 T T T  
0.4846025940450185 0.4692784690535052 0.6281171458992805 T T T  
0.0604748799763710 0.5392333283696145 0.6127998601265277 T T T  
0.5601162204317284 0.9540644937731471 0.6074549227019920 T T T  
0.9779736496181984 0.0303427726898728 0.6337504950328214 T T T  
0.1437852491133543 0.0375732283310478 0.5792523853456669 T T T  
0.4104728149061494 0.9479224134628045 0.6647809677157843 T T T  
0.8954562262510136 0.5383418192757178 0.6631813720562928 T T T  
0.6423364089279241 0.4815902159895224 0.5770554882308990 T T T  
0.0892730356860904 0.6922155380621902 0.7035923762417834 T T T  
0.3638465081023545 0.4283713977436382 0.7021484429354403 T T T  
0.8467939630490047 0.0691252967105379 0.7014051997549215 T T T  
0.5672488165040545 0.7711126483712945 0.6916499335758595 T T T  
0.2780934661051347 0.9247963508415633 0.3008164828263150 T T T  
0.5640886312423720 0.1807183734506253 0.3044112279930121 T T T  
0.7700506912860131 0.5627558690853912 0.3001742128750406 T T T  
0.0346161295789431 0.3127903303958597 0.2993952756756006 T T T  
0.0948527916315717 0.5091843073075019 0.6939750213685297 T T T  
0.3705354372451834 0.2433841909394422 0.6923567938771870 T T T  
0.9033396215152193 0.0247737704666691 0.7183436128806802 T T T  
0.6143482246708357 0.9086727419317243 0.6953480023253754 T T T  
0.1496456799006805 0.7291489622238104 0.7178707553737662 T T T

0.4243712116538678	0.4703808756984703	0.7158309653551144	T	T	T
0.8560268236388049	0.2539810856557496	0.6917074998414459	T	T	T
0.5040699005509014	0.8638651269875033	0.6830763452472834	T	T	T
0.2221499976509890	0.9691438593975333	0.2834265115255762	T	T	T
0.2682604112119865	0.7401069761602916	0.3107671702428745	T	T	T
0.5189277816971956	0.0365067040231661	0.3039631203997534	T	T	T
0.6250157382150676	0.0971853283720419	0.3158904359737393	T	T	T
0.7594328267796551	0.7449058669266060	0.3119184815411160	T	T	T
0.7122782750522745	0.5218701157136774	0.2838679107861477	T	T	T
0.0287422977826481	0.4954805909975084	0.3092660930633121	T	T	T
0.9742552615602841	0.2757732280036317	0.2851162459423487	T	T	T
0.6038708492392683	0.6334114254523524	0.6314314625289960	T	T	T
0.6487817750305567	0.6455289705310605	0.5195024736345744	F	F	F
0.6891918066408718	0.8622751359040890	0.3967411209772013	T	T	T

=====Fe Structures=====

Ti O Ti O Ti O

1.0000000000000000

14.2453041077000009 0.0000000000000000 0.0000000000000000

0.0000000000000000 5.1680002212999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 29.4789562224999990

Ti O H Fe

21 57 18 3

Selective dynamics

Direct

0.0212466977668545	0.1100294222427322	0.3677138729247342	T	T	T
0.1834650872785853	0.6318844698206824	0.3963119163804945	T	T	T
0.5204716042934594	0.3980290434811770	0.3641867815935644	T	T	T
0.7672593283392228	0.3486412410783693	0.3627037796352914	T	T	T

0.9341209914325401 0.6372139433923250 0.3974184499088484 T T T  
0.4388101978726843 0.8624387409160720 0.3992031555486171 T T T  
0.2723501137236860 0.1561547901574962 0.3640251874810252 T T T  
0.7342005810289152 0.1367530326270341 0.4848529224897646 F F F  
0.3956158154875027 0.8683481241609385 0.5172283169192724 F F F  
0.8953822014665107 0.6325289816178099 0.5172296942882255 F F F  
0.2344372928950307 0.3634625181788707 0.4844606095791164 F F F  
0.4815241771643173 0.3615968561732217 0.4834047030315531 F F F  
0.1487325421792534 0.8563983739423122 0.5193773182996253 F F F  
0.9814354254124780 0.1396032612863678 0.4834948480823442 F F F  
0.4444664571884219 0.1356488126091112 0.6059129352302957 T T T  
0.1076699635634293 0.8937318500927611 0.6383754975579776 T T T  
0.9435952813634448 0.3669733369881719 0.6061982961711871 T T T  
0.1867223709704892 0.3653356402801293 0.6049541860673877 T T T  
0.3566530817615424 0.6537494321053093 0.6369281862664358 T T T  
0.8556669105396419 0.8446722231169311 0.6384832379133755 T T T  
0.6881447713526162 0.1358422251967784 0.6027392915356693 T T T  
0.6699124544663578 0.1110836173668310 0.7319510058576534 T T T  
0.9698371568783708 0.8193894932188529 0.3418738351509130 T T T  
0.7447700878261616 0.1723181320979061 0.4191277765136592 T T T  
0.2508774772686674 0.3125496690685757 0.4211153307549454 T T T  
0.4695918289495948 0.6866750002000731 0.3411871811018812 T T T  
0.8047109750083655 0.7028318028644057 0.3954118554258873 T T T  
0.9014907283324739 0.3179968411503820 0.3657237442732484 T T T  
0.4077292053476368 0.1784327431875809 0.3634074828370746 T T T  
0.3098777305671197 0.8129709620617518 0.3965050942763777 T T T  
0.0661745797372847 0.4641596520963427 0.3898824873117366 T T T  
0.6468453097103075 0.5478177246529476 0.3699106849052483 T T T  
0.1481251085015627 0.9659858663963612 0.3691128157340871 T T T

0.5730661692826431 0.0224822237433611 0.3916751072119973 T T T  
0.7294901397141985 0.0823799543993437 0.3279087309017177 T T T  
0.9852943610686231 0.9652473829824438 0.4239507601725966 T T T  
0.4851898797813220 0.5304135763582534 0.4229624947677804 T T T  
0.2304954458006738 0.4592816446500594 0.3391553063063809 T T T  
0.6690919997630900 0.8170932275262288 0.4621108699766978 F F F  
0.4563443067348629 0.1856957460417874 0.5415381954083784 F F F  
0.9563715435325619 0.3157762323396867 0.5415514049333012 F F F  
0.1684768759925106 0.6845410757490313 0.4614047933963619 F F F  
0.5163401794135183 0.6840621747006708 0.5172222351935218 F F F  
0.6122121268392959 0.3153938228045661 0.4863254931615089 F F F  
0.1121104352761861 0.1862923125396918 0.4862169103188876 F F F  
0.0164653504910319 0.8169379209085434 0.5170864510602016 F F F  
0.7737086930159478 0.4642121896258828 0.5098542901532497 F F F  
0.3547568199701061 0.5398845750144545 0.4913055491984935 F F F  
0.8548352112812623 0.9612879754852131 0.4913474116743402 F F F  
0.2736558171006749 0.0367285287095171 0.5095842622449496 F F F  
0.4364578605973435 0.0348585244096000 0.4598389770138454 F F F  
0.6931547229194095 0.9653791778681509 0.5438751113830449 F F F  
0.1930960752500894 0.5368671613790212 0.5435284188581946 F F F  
0.9363025789852344 0.4660265976351923 0.4598071447971463 F F F  
0.3735825313454557 0.8185033598004056 0.5813247616349656 T T T  
0.1567112107723987 0.1880720675547526 0.6617202958187989 T T T  
0.6563229395785343 0.3417524366802306 0.6581032293759110 T T T  
0.8750037516764245 0.6836687488589810 0.5818228510714601 T T T  
0.2239171594074747 0.6844511457831038 0.6409351707722920 T T T  
0.3203503135161574 0.3125560934822549 0.6093555795288315 T T T  
0.8179960495886164 0.1835295386623599 0.6070710538966438 T T T  
0.7182506078156062 0.8223624427783506 0.6402791474002203 T T T



0.4858248991663885	0.4682745874991844	0.6282032836931231	T	T	T
0.0618659816097783	0.5353983112865814	0.6101384094290409	T	T	T
0.5623406250119206	0.9496198844726239	0.6109254065320855	T	T	T
0.9790141576234984	0.0335255326661722	0.6340766483101878	T	T	T
0.1445461409518466	0.0336523417309976	0.5800087689144314	T	T	T
0.4087113771818829	0.9494224081648719	0.6644643794855788	T	T	T
0.9031060137677117	0.5433170233191417	0.6644018917063039	T	T	T
0.6432851007902979	0.4799021264152182	0.5798844744721956	T	T	T
0.0696794588588339	0.6791777671876298	0.6988950471025209	T	T	T
0.3667074383983954	0.4321440589595736	0.7018085441396069	T	T	T
0.8500762778379998	0.0653628885572888	0.7014015371363556	T	T	T
0.5596768037411270	0.7373844630413473	0.6961680228172714	T	T	T
0.2774506925781812	0.9239459324165538	0.3011615558123069	T	T	T
0.5591051507936189	0.1855543678967992	0.3038516227980028	T	T	T
0.7798419467479523	0.6026955060777600	0.3016088630745976	T	T	T
0.0323685481620681	0.3140318795306884	0.2998179937838217	T	T	T
0.0033004672935026	0.6227846788831181	0.6921316393369793	T	T	T
0.3708142239108413	0.2454519008685309	0.6928751261384322	T	T	T
0.8677936412981356	0.2463769959066599	0.6933801014486786	T	T	T
0.6036999292758284	0.8634054116528652	0.7109241771039146	T	T	T
0.1066330176912527	0.5180770921337013	0.6968277566810706	T	T	T
0.4289848387497113	0.4738326922102125	0.7137453537901480	T	T	T
0.7871953162731024	0.0750640088684349	0.7160866751021022	T	T	T
0.5017869321585628	0.8429993138142096	0.6865949771315988	T	T	T
0.2219937654895705	0.9669949360991675	0.2833174754192091	T	T	T
0.2676904809587908	0.7391970701564925	0.3111638990285006	T	T	T
0.5216202989662718	0.0257408851533928	0.3061160242963297	T	T	T
0.6271318304260285	0.1287232227169325	0.3102465594789908	T	T	T
0.7669102473846958	0.7897307825087079	0.3102817613628662	T	T	T

0.7295641439313826	0.5549176313034961	0.2808506966213474	T	T	T
0.0250424714312677	0.4963016741751035	0.3097840480288888	T	T	T
0.9726216493033669	0.2742432065185975	0.2851622034716137	T	T	T
0.6586028852654016	0.2326019711103043	0.7043897493010177	T	T	T
0.6533134171089597	0.2064857692518933	0.7591927167510533	T	T	T
0.6063919353704689	0.6224707746839707	0.6333310624603303	T	T	T
0.6487817750305567	0.6455289705310605	0.5195024736345744	F	F	F
0.6826607271771096	0.8603486461747208	0.3988303658203661	T	T	T

Ti O Ti O Ti O

1.0000000000000000		
14.2453041077000009	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.1680002212999998	0.0000000000000000
0.0000000000000000	0.0000000000000000	29.4789562224999990

Ti O H Fe

21 57 17 3

Selective dynamics

Direct

0.0212080924707640	0.1089102064712967	0.3673577223053592	T	T	T
0.1831326739461478	0.6319185546356700	0.3965339428236744	T	T	T
0.5199483109244495	0.4006093643638420	0.3641744342520709	T	T	T
0.7677379632246792	0.3503578852632868	0.3625728813507221	T	T	T
0.9346356456451940	0.6368950260622790	0.3977343117768025	T	T	T
0.4381235243164338	0.8639988670952222	0.3993580295559972	T	T	T
0.2719446288240560	0.1574040093320774	0.3637797970811633	T	T	T
0.7342005810289152	0.1367530326270341	0.4848529224897646	F	F	F
0.3956158154875027	0.8683481241609385	0.5172283169192724	F	F	F
0.8953822014665107	0.6325289816178099	0.5172296942882255	F	F	F
0.2344372928950307	0.3634625181788707	0.4844606095791164	F	F	F

0.4815241771643173 0.3615968561732217 0.4834047030315531 F F F  
0.1487325421792534 0.8563983739423122 0.5193773182996253 F F F  
0.9814354254124780 0.1396032612863678 0.4834948480823442 F F F  
0.4425109546751356 0.1408666188586135 0.6061435731096249 T T T  
0.1071418794521241 0.8953003048853730 0.6380843004248331 T T T  
0.9432831667702520 0.3728347779660087 0.6064427259427871 T T T  
0.1867142794036535 0.3670888907963774 0.6054570927795359 T T T  
0.3568466767599145 0.6600787496323447 0.6373426720927301 T T T  
0.8554850171855086 0.8509641557384442 0.6388412756994055 T T T  
0.6878783252006435 0.1459108522934842 0.6023636809069394 T T T  
0.6808640375849911 0.0803943469920785 0.7340195301151399 T T T  
0.9700125462634437 0.8183251217134355 0.3417218485065662 T T T  
0.7445511243852788 0.1714201416153699 0.4189318578429949 T T T  
0.2508045859933304 0.3131846491151231 0.4209262740802501 T T T  
0.4698730242221703 0.6891776408744329 0.3410962138570822 T T T  
0.8050525978213288 0.7025780887229029 0.3954990153785140 T T T  
0.9012645239564714 0.3178209012309372 0.3656989609547298 T T T  
0.4078260797999633 0.1799894379209835 0.3635157425716501 T T T  
0.3098706642560418 0.8131868612048866 0.3964642271965924 T T T  
0.0660936017519245 0.4639847975485912 0.3898585156348476 T T T  
0.6471393193084465 0.5517040906857612 0.3702949383073094 T T T  
0.1481874684884990 0.9662685251558045 0.3690312716467219 T T T  
0.5734357191453170 0.0235044890826500 0.3919344429852292 T T T  
0.7292151407918720 0.0812704017877825 0.3284339794215452 T T T  
0.9852582001054300 0.9651338387044364 0.4237179551550814 T T T  
0.4852712630580490 0.5316303319431722 0.4228985720161914 T T T  
0.2305299040214932 0.4601007606639722 0.3389808893623876 T T T  
0.6690919997630900 0.8170932275262288 0.4621108699766978 F F F  
0.4563443067348629 0.1856957460417874 0.5415381954083784 F F F

0.9563715435325619	0.3157762323396867	0.5415514049333012	F	F	F
0.1684768759925106	0.6845410757490313	0.4614047933963619	F	F	F
0.5163401794135183	0.6840621747006708	0.5172222351935218	F	F	F
0.6122121268392959	0.3153938228045661	0.4863254931615089	F	F	F
0.1121104352761861	0.1862923125396918	0.4862169103188876	F	F	F
0.0164653504910319	0.8169379209085434	0.5170864510602016	F	F	F
0.7737086930159478	0.4642121896258828	0.5098542901532497	F	F	F
0.3547568199701061	0.5398845750144545	0.4913055491984935	F	F	F
0.8548352112812623	0.9612879754852131	0.4913474116743402	F	F	F
0.2736558171006749	0.0367285287095171	0.5095842622449496	F	F	F
0.4364578605973435	0.0348585244096000	0.4598389770138454	F	F	F
0.6931547229194095	0.9653791778681509	0.5438751113830449	F	F	F
0.1930960752500894	0.5368671613790212	0.5435284188581946	F	F	F
0.9363025789852344	0.4660265976351923	0.4598071447971463	F	F	F
0.3729620632836684	0.8202342095113926	0.5807273867361946	T	T	T
0.1565198264082985	0.1896270538374374	0.6615213854166508	T	T	T
0.6556242005879923	0.3529166891836222	0.6565371093164337	T	T	T
0.8757123400211723	0.6886931482855446	0.5811065261674307	T	T	T
0.2236851016190772	0.6865587474495723	0.6412105146772025	T	T	T
0.3195301074340684	0.3178316184422270	0.6088958647248595	T	T	T
0.8172933792127701	0.1899149343250862	0.6061119021097902	T	T	T
0.7186532914845410	0.8282723045674941	0.6382958847627572	T	T	T
0.4850550360008980	0.4749738914641903	0.6254371068515521	T	T	T
0.0618175029908866	0.5391181993472435	0.6099797778643288	T	T	T
0.5623243349984951	0.9576326409752516	0.6107779703849461	T	T	T
0.9788066021802012	0.0379291218820731	0.6336306280064222	T	T	T
0.1446886331993204	0.0347106460194495	0.5797356474601049	T	T	T
0.4063142168511768	0.9606755667260367	0.6631995067516182	T	T	T
0.9026634996989125	0.5474818224557642	0.6636172918755127	T	T	T

0.6438084491692896	0.4853796380183530	0.5765498306140686	T	T	T
0.0690068867048511	0.6866037728922758	0.6989878363721173	T	T	T
0.3768682711958183	0.4518107666515132	0.7014890815515794	T	T	T
0.8464517397925955	0.0555930171233134	0.7003415451265902	T	T	T
0.5646392542035650	0.7289848643274369	0.6927753745279517	T	T	T
0.2784828371977928	0.9237581215426316	0.3012621478252616	T	T	T
0.5591210259028375	0.1873096640671348	0.3041038550442285	T	T	T
0.7797215701333957	0.6028752264913475	0.3017080634865564	T	T	T
0.0324389123880942	0.3152130408063289	0.2999597326977933	T	T	T
0.0027503265458936	0.6289363350532189	0.6928276359897482	T	T	T
0.3786993976913327	0.2631088252215593	0.6943767382298937	T	T	T
0.8650064695311516	0.2376920871622183	0.6951413102870059	T	T	T
0.6440506799558521	0.9289379549178327	0.7228841761801272	T	T	T
0.1061745980908779	0.5258816520943281	0.6981637807342063	T	T	T
0.4415323375324645	0.4976026407584684	0.7103011422621999	T	T	T
0.7806216461367458	0.0577658638150030	0.7157894090740248	T	T	T
0.5126669158783745	0.8538262129589602	0.6863580854129595	T	T	T
0.2248027430799621	0.9673923443611814	0.2822428893347415	T	T	T
0.2677030952315848	0.7392201326788991	0.3111695344380405	T	T	T
0.5211644381599526	0.0282249812451892	0.3060386289132702	T	T	T
0.6269004271791738	0.1290326423421028	0.3105237144880808	T	T	T
0.7667870041385630	0.7899104427831483	0.3103747474293946	T	T	T
0.7307204549836297	0.5562422023832180	0.2801730675908838	T	T	T
0.0237256551499136	0.4973409882043102	0.3098135254002365	T	T	T
0.9740995540726690	0.2732332834622046	0.2842316160408984	T	T	T
0.6604187102628358	0.2193788357658141	0.7131693665099067	T	T	T
0.6050619128442211	0.6342945949298147	0.6346004523095105	T	T	T
0.6487817750305567	0.6455289705310605	0.5195024736345744	F	F	F
0.6830977798600197	0.8631366190193388	0.3987685912843734	T	T	T

Ti O H Co

1.0000000000000000

14.2453041077000009 0.0000000000000000 0.0000000000000000

0.0000000000000000 5.1680002212999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 29.4789562224999990

Ti O H Fe

21 57 17 3

Selective dynamics

Direct

0.0215486144738944 0.1116503927107489 0.3678489592214321 T T T

0.1840131380637126 0.6323068841400831 0.3959845847519277 T T T

0.5212292235695846 0.3967434674766920 0.3643837371091102 T T T

0.7673232509212923 0.3510019399616993 0.3624725984034407 T T T

0.9341133369333610 0.6383880834215763 0.3972692339492348 T T T

0.4398155400979704 0.8621548249789532 0.3989155942606455 T T T

0.2729556082885925 0.1554509935407704 0.3642084040749362 T T T

0.7342005810289152 0.1367530326270341 0.4848529224897646 F F F

0.3956158154875027 0.8683481241609385 0.5172283169192724 F F F

0.8953822014665107 0.6325289816178099 0.5172296942882255 F F F

0.2344372928950307 0.3634625181788707 0.4844606095791164 F F F

0.4815241771643173 0.3615968561732217 0.4834047030315531 F F F

0.1487325421792534 0.8563983739423122 0.5193773182996253 F F F

0.9814354254124780 0.1396032612863678 0.4834948480823442 F F F

0.4481017592710316 0.1428645515248597 0.6049786346976062 T T T

0.1064013310228531 0.8989415493294911 0.6390032241937088 T T T

0.9414104919401587 0.3710512956645009 0.6057406436819335 T T T

0.1825810994008175 0.3692093977204047 0.6044519209809717 T T T

0.3538290478224365 0.6394873672312282 0.6353148562250640 T T T

0.8550951356102002	0.8509072790749288	0.6387302410428131	T	T	T
0.6889915240925664	0.1336989586846444	0.5997544914365309	T	T	T
0.6089901459025446	0.9240434762322663	0.7193338453182648	T	T	T
0.9702698419516704	0.8207888548080582	0.3419729621326757	T	T	T
0.7448651188346582	0.1737345165574870	0.4190075419257886	T	T	T
0.2512486608854969	0.3125408152727425	0.4213316902247720	T	T	T
0.4698927328309017	0.6859516244463654	0.3413512630235248	T	T	T
0.8051871675209467	0.7054559358849061	0.3952815089336539	T	T	T
0.9018084351001177	0.3191053973757219	0.3658369528551249	T	T	T
0.4078549041524103	0.1789774103294230	0.3633474507983072	T	T	T
0.3101756240915255	0.8139005908033484	0.3964741817751320	T	T	T
0.0665867036371787	0.4648066409369612	0.3899291039201748	T	T	T
0.6469999860349468	0.5494134186913124	0.3699279944485762	T	T	T
0.1483043718246702	0.9663418257104393	0.3691799404383494	T	T	T
0.5727565725310544	0.0251508252373174	0.3915784387394832	T	T	T
0.7301924435935445	0.0884153888313151	0.3269743901624566	T	T	T
0.9855626099972421	0.9664120543273543	0.4241216183460092	T	T	T
0.4851572869822920	0.5303558329405713	0.4230552446199708	T	T	T
0.2307083307493498	0.4592963898684446	0.3393670130122231	T	T	T
0.6690919997630900	0.8170932275262288	0.4621108699766978	F	F	F
0.4563443067348629	0.1856957460417874	0.5415381954083784	F	F	F
0.9563715435325619	0.3157762323396867	0.5415514049333012	F	F	F
0.1684768759925106	0.6845410757490313	0.4614047933963619	F	F	F
0.5163401794135183	0.6840621747006708	0.5172222351935218	F	F	F
0.6122121268392959	0.3153938228045661	0.4863254931615089	F	F	F
0.1121104352761861	0.1862923125396918	0.4862169103188876	F	F	F
0.0164653504910319	0.8169379209085434	0.5170864510602016	F	F	F
0.7737086930159478	0.4642121896258828	0.5098542901532497	F	F	F
0.3547568199701061	0.5398845750144545	0.4913055491984935	F	F	F

0.8548352112812623 0.9612879754852131 0.4913474116743402 F F F  
0.2736558171006749 0.0367285287095171 0.5095842622449496 F F F  
0.4364578605973435 0.0348585244096000 0.4598389770138454 F F F  
0.6931547229194095 0.9653791778681509 0.5438751113830449 F F F  
0.1930960752500894 0.5368671613790212 0.5435284188581946 F F F  
0.9363025789852344 0.4660265976351923 0.4598071447971463 F F F  
0.3741639830181620 0.8235588418217962 0.5825083267280222 T T T  
0.1564532536906626 0.1920563708583093 0.6619029059452278 T T T  
0.6643928598608473 0.3297242500185631 0.6624994602713583 T T T  
0.8752044064398904 0.6876835531604523 0.5822532115323962 T T T  
0.2233531218391993 0.6885614441156583 0.6404801961134443 T T T  
0.3201650826734181 0.3119666168225625 0.6098902251476878 T T T  
0.8185829640158211 0.1891278115432138 0.6057671632153731 T T T  
0.7192892084229110 0.8241437323288187 0.6407382975263424 T T T  
0.4852039150373902 0.4646600578598067 0.6312869545050612 T T T  
0.0616304575436860 0.5396646913169939 0.6099458230566316 T T T  
0.5624185420621146 0.9555204609384274 0.6123636314945675 T T T  
0.9780739173436588 0.0420848899614670 0.6362520345018885 T T T  
0.1426563698371110 0.0369159046444304 0.5803081342254972 T T T  
0.4081760763140482 0.9536039019608253 0.6669878308464587 T T T  
0.9052041792527786 0.5559439437186368 0.6649967017849712 T T T  
0.6431746318287422 0.4768780669545575 0.5823698093112102 T T T  
0.0701257989361528 0.6824869200678504 0.6989976413929992 T T T  
0.3604652474560042 0.4406640634335146 0.7026326229597429 T T T  
0.8271958708981463 0.1090268884679630 0.6982196645987152 T T T  
0.5621580313666653 0.7151683049375706 0.6954852702142372 T T T  
0.2778118743871474 0.9245570556198560 0.3012006426270789 T T T  
0.5590863165211047 0.1873834130280866 0.3036117941100848 T T T  
0.7807719301049074 0.6075058761675197 0.3017637757624237 T T T



0.0326333430878442	0.3140551423470972	0.2999045933245150	T	T	T
0.0039649726722367	0.6239795826066150	0.6914691200017467	T	T	T
0.3674464084670866	0.2533944397290516	0.6949793017302384	T	T	T
0.8713691348261959	0.2571080226187555	0.6953571571794525	T	T	T
0.1080572331412868	0.5230088020106823	0.6974103065551763	T	T	T
0.4200698107273183	0.4890328570591183	0.7167460283490500	T	T	T
0.7673358926266042	0.1954059346232357	0.6890251517080135	T	T	T
0.4672309358421991	0.8869935665057767	0.6817232888230158	T	T	T
0.2223790964853724	0.9675446002608170	0.2833276781716185	T	T	T
0.2682547751252705	0.7396984343536586	0.3110868422616566	T	T	T
0.5221268311802997	0.0267116616126400	0.3058134103895165	T	T	T
0.6274421529181554	0.1321314596459033	0.3096259672193223	T	T	T
0.7674464025626501	0.7948546069066125	0.3101067543895563	T	T	T
0.7317965966630842	0.5588758481474918	0.2803567542676642	T	T	T
0.0249199768597044	0.4965289712844055	0.3096687349438434	T	T	T
0.9731135786549108	0.2728035979339650	0.2851464439898627	T	T	T
0.6191115289666075	0.2323491599658640	0.6810756550714231	T	T	T
0.6733909235240549	0.8571631816254945	0.7218943447708029	T	T	T
0.6069008388092054	0.6330246310740613	0.6354272380035773	T	T	T
0.6487817750305567	0.6455289705310605	0.5195024736345744	F	F	F
0.6827878152879832	0.8617461527226200	0.3990829823259733	T	T	T

Ti O H Co

1.0000000000000000

14.2453041077000009 0.0000000000000000 0.0000000000000000

0.0000000000000000 5.1680002212999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 29.4789562224999990

Ti O H Fe

21 57 16 3

## Selective dynamics

### Direct

0.0223911201174828	0.1112217268292522	0.3674794838201809	T	T	T
0.1861429115248692	0.6338139969882473	0.3960784239560144	T	T	T
0.5236989367724448	0.3943138713996631	0.3665616928145524	T	T	T
0.7672925865569505	0.3523794765506940	0.3657490687808560	T	T	T
0.9369271672120715	0.6366403284542206	0.3972705667910773	T	T	T
0.4424478713177110	0.8649757934945965	0.3980665538960906	T	T	T
0.2737944677523714	0.1555010019244184	0.3642240666950008	T	T	T
0.7342005810289152	0.1367530326270341	0.4848529224897646	F	F	F
0.3956158154875027	0.8683481241609385	0.5172283169192724	F	F	F
0.8953822014665107	0.6325289816178099	0.5172296942882255	F	F	F
0.2344372928950307	0.3634625181788707	0.4844606095791164	F	F	F
0.4815241771643173	0.3615968561732217	0.4834047030315531	F	F	F
0.1487325421792534	0.8563983739423122	0.5193773182996253	F	F	F
0.9814354254124780	0.1396032612863678	0.4834948480823442	F	F	F
0.4462751476762801	0.1514457163688133	0.6051231205144308	T	T	T
0.1050424663807828	0.9003202854752853	0.6382130338072706	T	T	T
0.9414852113149333	0.3749244602625647	0.6061036335161452	T	T	T
0.1834169180907366	0.3711283741707184	0.6050801530663366	T	T	T
0.3541453505227872	0.6518638499526063	0.6359291611120226	T	T	T
0.8521076204808636	0.8552407613522445	0.6377703157763752	T	T	T
0.6871245159791383	0.1526545251705620	0.5995558904551173	T	T	T
0.5554467179557799	0.9690651648602138	0.7087511053646490	T	T	T
0.9698008667739499	0.8208747076878719	0.3416498541205684	T	T	T
0.7483717441981436	0.1739088765733847	0.4209532108379899	T	T	T
0.2516593663081426	0.3135819907436024	0.4211861489789053	T	T	T
0.4738768181603949	0.6862338005189200	0.3420786369367576	T	T	T
0.8055368646641633	0.6914290217800982	0.3968756679694135	T	T	T

0.9005212728654474	0.3190429527899622	0.3646263257496402	T	T	T
0.4083273506240634	0.1819337774461110	0.3630268019929048	T	T	T
0.3102996903008070	0.8160317932105476	0.3960853815724741	T	T	T
0.0661954356325237	0.4643806021991771	0.3898257771484502	T	T	T
0.6480473095173456	0.5476926363593926	0.3736361599119880	T	T	T
0.1480122434282136	0.9668176499094050	0.3689869170426687	T	T	T
0.5715413673162695	0.0350778571264620	0.3943079894525192	T	T	T
0.7214537324176646	0.0392685700539406	0.3401576270503903	T	T	T
0.9848575894932159	0.9663506879470702	0.4236436404162559	T	T	T
0.4843431059716545	0.5334409909235471	0.4238541326434657	T	T	T
0.2305705042172354	0.4596149879487634	0.3393475079117745	T	T	T
0.6690919997630900	0.8170932275262288	0.4621108699766978	F	F	F
0.4563443067348629	0.1856957460417874	0.5415381954083784	F	F	F
0.9563715435325619	0.3157762323396867	0.5415514049333012	F	F	F
0.1684768759925106	0.6845410757490313	0.4614047933963619	F	F	F
0.5163401794135183	0.6840621747006708	0.5172222351935218	F	F	F
0.6122121268392959	0.3153938228045661	0.4863254931615089	F	F	F
0.1121104352761861	0.1862923125396918	0.4862169103188876	F	F	F
0.0164653504910319	0.8169379209085434	0.5170864510602016	F	F	F
0.7737086930159478	0.4642121896258828	0.5098542901532497	F	F	F
0.3547568199701061	0.5398845750144545	0.4913055491984935	F	F	F
0.8548352112812623	0.9612879754852131	0.4913474116743402	F	F	F
0.2736558171006749	0.0367285287095171	0.5095842622449496	F	F	F
0.4364578605973435	0.0348585244096000	0.4598389770138454	F	F	F
0.6931547229194095	0.9653791778681509	0.5438751113830449	F	F	F
0.1930960752500894	0.5368671613790212	0.5435284188581946	F	F	F
0.9363025789852344	0.4660265976351923	0.4598071447971463	F	F	F
0.3732905200149776	0.8292778082982516	0.5821891228894504	T	T	T
0.1560941923015267	0.1931964219648350	0.6615470040182284	T	T	T

0.6564597765010889 0.3325319056129370 0.6601502859084397 T T T  
0.8757415931473225 0.6920068837139827 0.5811273130891004 T T T  
0.2224469797190598 0.6915807356705100 0.6404453798177000 T T T  
0.3196697812295803 0.3227485897719048 0.6092023737472719 T T T  
0.8172217491945323 0.1954577893677961 0.6051979765511035 T T T  
0.7196209996022650 0.8265590689955111 0.6380295045817252 T T T  
0.4838277937677022 0.4757648011227040 0.6301568971969050 T T T  
0.0612366324706950 0.5432198071437224 0.6097412358924096 T T T  
0.5607632410665188 0.9631380256062295 0.6123920008729358 T T T  
0.9777013481333815 0.0447811885857209 0.6348249073961664 T T T  
0.1431657989063679 0.0386596383404549 0.5798274579421920 T T T  
0.4023476441605537 0.9702004686990414 0.6661175255857639 T T T  
0.9023513359732874 0.5558845168967687 0.6638875796924693 T T T  
0.6428364677219742 0.4794350157842359 0.5771814145235005 T T T  
0.0678947354975591 0.6880145913748261 0.6986798466592036 T T T  
0.3558209000578413 0.4511619923361671 0.7024279482086112 T T T  
0.8356001772955765 0.0999568979721874 0.6984815695491229 T T T  
0.5815643537526382 0.7256007008562361 0.6967918647167253 T T T  
0.2783340079185465 0.9243574779940029 0.3011547001597850 T T T  
0.5639907855092716 0.1864271360313887 0.3047787454328690 T T T  
0.7694781218102322 0.5814594146632996 0.3017599396565067 T T T  
0.0336928323845159 0.3149791517793970 0.2997900897705021 T T T  
0.0017202869062457 0.6296614323881040 0.6916703854450221 T T T  
0.3578078561632443 0.2638173362561094 0.6941198002230948 T T T  
0.8636968457014204 0.2728630295096968 0.6910450768737157 T T T  
0.1055322752069819 0.5281083947503383 0.6976950348656116 T T T  
0.4146870634022261 0.4850251128540609 0.7183225689804695 T T T  
0.7683218756657179 0.1381511186360518 0.7006160584245702 T T T  
0.4624291965577434 0.9701595806001330 0.6861274497257054 T T T

0.2233750037172239	0.9688059292212295	0.2830602181643316	T	T	T
0.2680309844112491	0.7397191885955061	0.3110601242543315	T	T	T
0.5199228436788708	0.0397988868761527	0.3042794337730494	T	T	T
0.6260504086708114	0.1067522609196816	0.3156728215937290	T	T	T
0.7588068742071997	0.7641609523103197	0.3135023693385290	T	T	T
0.7133869045376009	0.5426155794322213	0.2840251787320856	T	T	T
0.0263174843506484	0.4972391329837675	0.3097218588020771	T	T	T
0.9744474822855288	0.2752379475604254	0.2847039663530671	T	T	T
0.6125768579068334	0.2268893019658459	0.6791824459843429	T	T	T
0.6043097889893420	0.6459241151216484	0.6367701490639794	T	T	T
0.6487817750305567	0.6455289705310605	0.5195024736345744	F	F	F
0.6860807341970615	0.8739221695277215	0.3995756543391910	T	T	T

Ti O H Co

1.000000000000000		
14.2453041077000009	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.1680002212999998	0.0000000000000000
0.0000000000000000	0.0000000000000000	29.4789562224999990

Ti O H Fe

21 57 15 3

Selective dynamics

Direct

0.0209911936839600	0.1078968377819483	0.3672404093733594	T	T	T
0.1827386519597443	0.6316287326586167	0.3966366841579622	T	T	T
0.5192213280762805	0.4035773667140363	0.3640136976162421	T	T	T
0.7676653104860582	0.3496518546090616	0.3628773773983188	T	T	T
0.9346930827562480	0.6361326423044190	0.3980204721605538	T	T	T
0.4373170395463229	0.8651102805579081	0.3999187103807958	T	T	T
0.2717793748074128	0.1579549350409342	0.3636896693005064	T	T	T

0.7342005810289152 0.1367530326270341 0.4848529224897646 F F F  
0.3956158154875027 0.8683481241609385 0.5172283169192724 F F F  
0.8953822014665107 0.6325289816178099 0.5172296942882255 F F F  
0.2344372928950307 0.3634625181788707 0.4844606095791164 F F F  
0.4815241771643173 0.3615968561732217 0.4834047030315531 F F F  
0.1487325421792534 0.8563983739423122 0.5193773182996253 F F F  
0.9814354254124780 0.1396032612863678 0.4834948480823442 F F F  
0.4407071408497054 0.1462660108441131 0.6064421819452229 T T T  
0.1073151425934914 0.8976592562156475 0.6379748876746077 T T T  
0.9433627604307009 0.3721788137081704 0.6064525071654188 T T T  
0.1870923885056200 0.3702985185174958 0.6052909522459970 T T T  
0.3573895968154435 0.6682146551472459 0.6385048395824323 T T T  
0.8536558009977958 0.8526476513977868 0.6374462608306648 T T T  
0.6874885610575063 0.1494977689409534 0.5994821449068342 T T T  
0.5989468236853456 0.9561293357418467 0.7149089502082083 T T T  
0.9697042573065011 0.8175310657114571 0.3417044336059169 T T T  
0.7448090402402037 0.1711074474464584 0.4189857533537248 T T T  
0.2504987057703702 0.3132498146780963 0.4208268180121668 T T T  
0.4700893335684811 0.6920403135296990 0.3408944422732825 T T T  
0.8048267568690248 0.7010184991616477 0.3956808724817452 T T T  
0.9009789075111647 0.3177405032941603 0.3655895097738376 T T T  
0.4077067779594886 0.1802421739877589 0.3636013397764972 T T T  
0.3095543654252147 0.8130574537132655 0.3964417488713165 T T T  
0.0657764103859160 0.4636289114112682 0.3898423916169708 T T T  
0.6470937041131362 0.5520955682070071 0.3705237092720076 T T T  
0.1479383009838660 0.9661192578746017 0.3689312902799459 T T T  
0.5741303884736368 0.0225551797028966 0.3922162261340497 T T T  
0.7283193010512283 0.0762819551699289 0.3295312972334024 T T T  
0.9850753683439184 0.9648569435268191 0.4236588343094360 T T T

0.4846507940799670 0.5322772565265481 0.4226242319889349 T T T  
0.2303060571198279 0.4602168608077846 0.3388808049005400 T T T  
0.6690919997630900 0.8170932275262288 0.4621108699766978 F F F  
0.4563443067348629 0.1856957460417874 0.5415381954083784 F F F  
0.9563715435325619 0.3157762323396867 0.5415514049333012 F F F  
0.1684768759925106 0.6845410757490313 0.4614047933963619 F F F  
0.5163401794135183 0.6840621747006708 0.5172222351935218 F F F  
0.6122121268392959 0.3153938228045661 0.4863254931615089 F F F  
0.1121104352761861 0.1862923125396918 0.4862169103188876 F F F  
0.0164653504910319 0.8169379209085434 0.5170864510602016 F F F  
0.7737086930159478 0.4642121896258828 0.5098542901532497 F F F  
0.3547568199701061 0.5398845750144545 0.4913055491984935 F F F  
0.8548352112812623 0.9612879754852131 0.4913474116743402 F F F  
0.2736558171006749 0.0367285287095171 0.5095842622449496 F F F  
0.4364578605973435 0.0348585244096000 0.4598389770138454 F F F  
0.6931547229194095 0.9653791778681509 0.5438751113830449 F F F  
0.1930960752500894 0.5368671613790212 0.5435284188581946 F F F  
0.9363025789852344 0.4660265976351923 0.4598071447971463 F F F  
0.3759323376747289 0.8210968040220905 0.5813730179578983 T T T  
0.1569941104697343 0.1913341240083450 0.6614228065537960 T T T  
0.6593519722162414 0.3471891273675523 0.6592327127614307 T T T  
0.8745179818473890 0.6888535019631417 0.5812659976307158 T T T  
0.2227570219609930 0.6887792761291960 0.6407887399227539 T T T  
0.3199538022356304 0.3255762513941610 0.6075233514518019 T T T  
0.8173550753392890 0.1902023434339176 0.6056525690404142 T T T  
0.7166500430313355 0.8308107535916553 0.6393494131742837 T T T  
0.4865154040164583 0.4805140784126451 0.6305907757547348 T T T  
0.0610106225643485 0.5405708557934074 0.6099465581639375 T T T  
0.5620137905209831 0.9702058874484201 0.6118612133085651 T T T

0.9773592011857674	0.0401497142747220	0.6348046736723365	T	T	T
0.1436976209386562	0.0366875385005064	0.5796526727493062	T	T	T
0.3992394798132221	0.9727795718036567	0.6631177037520851	T	T	T
0.9012799015217775	0.5520304424163396	0.6639091584855201	T	T	T
0.6447077966638346	0.4848077867647610	0.5773858735446967	T	T	T
0.0681861086670003	0.6872808327195429	0.6987837562277583	T	T	T
0.3599744656672513	0.4416817074473502	0.7016019747813849	T	T	T
0.8374471797764856	0.0871782716666832	0.6995337010503919	T	T	T
0.5677368336460739	0.7472059896573783	0.6958947813533665	T	T	T
0.2780473966703239	0.9238456819686341	0.3012039946244160	T	T	T
0.5587862975491974	0.1847594653421895	0.3045420217712360	T	T	T
0.7783003960769961	0.5999569106734579	0.3015986034201174	T	T	T
0.0320122607591164	0.3159823067532564	0.2999260064846854	T	T	T
0.0020461626142169	0.6295076334879268	0.6920433597657520	T	T	T
0.3681337403383020	0.2549780746311231	0.6927963204883862	T	T	T
0.8586160722447203	0.2663382438661737	0.6915451572616104	T	T	T
0.1055428393257844	0.5268744974110826	0.6977375717727907	T	T	T
0.4163294126450368	0.4878014085604491	0.7186066305601987	T	T	T
0.7699932612821951	0.1025730506556667	0.7052148646112189	T	T	T
0.2239297806996675	0.9674845047073659	0.2824744749020445	T	T	T
0.2673593114607585	0.7393514790478762	0.3111952307459355	T	T	T
0.5206347233680545	0.0259218828578761	0.3069052158877487	T	T	T
0.6263700200218931	0.1260297198978930	0.3112007556463224	T	T	T
0.7657569486904997	0.7866906872015026	0.3106264850936376	T	T	T
0.7280756677453482	0.5543837845813959	0.2806546119047960	T	T	T
0.0235140535987409	0.4978295081093312	0.3100259890816181	T	T	T
0.9733088615581708	0.2749466039815528	0.2844375443242159	T	T	T
0.6187411409161612	0.2434116305888578	0.6795830214663271	T	T	T
0.6024145610743270	0.6511316155099740	0.6353837612192165	T	T	T



0.6487817750305567 0.6455289705310605 0.5195024736345744 F F F  
0.6832258801457417 0.8642443773525388 0.3986825211075318 T T T

Ti O H Co

1.0000000000000000

14.2453041077000009 0.0000000000000000 0.0000000000000000

0.0000000000000000 5.1680002212999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 29.4789562224999990

Ti O H Fe

21 55 15 3

Selective dynamics

Direct

0.0213385592815088 0.1098929671062868 0.3675724391739336 T T T

0.1834385372293787 0.6322877243476732 0.3962506285590735 T T T

0.5214024901878274 0.4025673531188743 0.3647871411825707 T T T

0.7666359641378462 0.3501456669415984 0.3636208396196028 T T T

0.9343179826302455 0.6372408988447247 0.3976546199283241 T T T

0.4386710121282257 0.8649995759682028 0.3994761304462679 T T T

0.2729596062858163 0.1573269183623220 0.3640109691385430 T T T

0.7342005810289152 0.1367530326270341 0.4848529224897646 F F F

0.3956158154875027 0.8683481241609385 0.5172283169192724 F F F

0.8953822014665107 0.6325289816178099 0.5172296942882255 F F F

0.2344372928950307 0.3634625181788707 0.4844606095791164 F F F

0.4815241771643173 0.3615968561732217 0.4834047030315531 F F F

0.1487325421792534 0.8563983739423122 0.5193773182996253 F F F

0.9814354254124780 0.1396032612863678 0.4834948480823442 F F F

0.4386152974469211 0.1488057658817074 0.6059199792890456 T T T

0.1079503768807932 0.9005131754858249 0.6382268201280752 T T T

0.9432405966193961 0.3736574790494217 0.6060777352790183 T T T

0.1859916562189463	0.3735199895325340	0.6049341819794847	T	T	T
0.3582023038923706	0.6692974342172507	0.6391579841579152	T	T	T
0.8546010099539499	0.8530349119298136	0.6383483403644880	T	T	T
0.6881708186526087	0.1382776819901681	0.5993651691548181	T	T	T
0.9695320433354113	0.8197678534864563	0.3418291227780607	T	T	T
0.7460267057287177	0.1733563565098238	0.4199039521924056	T	T	T
0.2508718913160428	0.3132704371718688	0.4210883881383023	T	T	T
0.4714826248951446	0.6913998404362585	0.3413348392162462	T	T	T
0.8049457596393417	0.7015458602616145	0.3961009363785532	T	T	T
0.9006859899680154	0.3190231088796774	0.3655204480937031	T	T	T
0.4080986924414514	0.1807750380352252	0.3636385000546026	T	T	T
0.3098851118389445	0.8140156072243506	0.3963610052159684	T	T	T
0.0660946155032090	0.4643045979869637	0.3898008815079038	T	T	T
0.6473253099644145	0.5482060188043563	0.3717714337091558	T	T	T
0.1480201094032005	0.9666359604949322	0.3690674013516550	T	T	T
0.5741108379865357	0.0255801368121447	0.3929874731405487	T	T	T
0.7268340276006714	0.0666439964453776	0.3322090634256660	T	T	T
0.9851495965357535	0.9660175059418747	0.4238551324076105	T	T	T
0.4841919014039654	0.5325473076842824	0.4230610956584764	T	T	T
0.2306359360490364	0.4602635726170398	0.3391528599312884	T	T	T
0.6690919997630900	0.8170932275262288	0.4621108699766978	F	F	F
0.4563443067348629	0.1856957460417874	0.5415381954083784	F	F	F
0.9563715435325619	0.3157762323396867	0.5415514049333012	F	F	F
0.1684768759925106	0.6845410757490313	0.4614047933963619	F	F	F
0.5163401794135183	0.6840621747006708	0.5172222351935218	F	F	F
0.6122121268392959	0.3153938228045661	0.4863254931615089	F	F	F
0.1121104352761861	0.1862923125396918	0.4862169103188876	F	F	F
0.0164653504910319	0.8169379209085434	0.5170864510602016	F	F	F
0.7737086930159478	0.4642121896258828	0.5098542901532497	F	F	F

0.3547568199701061 0.5398845750144545 0.4913055491984935 F F F  
0.8548352112812623 0.9612879754852131 0.4913474116743402 F F F  
0.2736558171006749 0.0367285287095171 0.5095842622449496 F F F  
0.4364578605973435 0.0348585244096000 0.4598389770138454 F F F  
0.6931547229194095 0.9653791778681509 0.5438751113830449 F F F  
0.1930960752500894 0.5368671613790212 0.5435284188581946 F F F  
0.9363025789852344 0.4660265976351923 0.4598071447971463 F F F  
0.3761955862935732 0.8224660673510291 0.5821504132598216 T T T  
0.1566830364618244 0.1946936922728297 0.6616113685659920 T T T  
0.6529741430472107 0.3469050813592443 0.6632958733542588 T T T  
0.8744314345792810 0.6899492615119401 0.5819616378391774 T T T  
0.2230166595178652 0.6909994278940289 0.6403692671313465 T T T  
0.3198519481940281 0.3232229867600241 0.6079317993739712 T T T  
0.8162889574952172 0.1937126575579560 0.6067208517558826 T T T  
0.7165802672204920 0.8259301764893928 0.6405003092972192 T T T  
0.4855275688137221 0.4789052897276723 0.6331069613081493 T T T  
0.0608910747247061 0.5422497032178837 0.6099231571989915 T T T  
0.5611398088048515 0.9657375202281671 0.6141034635215542 T T T  
0.9770974833002183 0.0428242764846800 0.6354385826663252 T T T  
0.1433103842120943 0.0389939907656795 0.5798742126306698 T T T  
0.4007139181469992 0.9694797700513575 0.6647493571446720 T T T  
0.9033844167668674 0.5559745121729883 0.6647397114698104 T T T  
0.6439045757137269 0.4696451618875290 0.5766737492649313 T T T  
0.0700232258878882 0.6861857486916612 0.6988169080611453 T T T  
0.3507515612656836 0.4292621592191332 0.7014764226981893 T T T  
0.8308922701407538 0.1035309477677093 0.6987926691775991 T T T  
0.2777098301007128 0.9249856869432767 0.3011977758812615 T T T  
0.5594404300963838 0.1833330456444609 0.3048319996985304 T T T  
0.7754302438678653 0.5955353670158893 0.3016588168140101 T T T

0.0323657768114332	0.3155284958772337	0.2999462484932972	T	T	T
0.0037187627104870	0.6292177118112419	0.6919351904544792	T	T	T
0.3626398457888114	0.2444668098455237	0.6918680788170144	T	T	T
0.8644839644952982	0.2695656733459568	0.6921812380412929	T	T	T
0.1073088915607461	0.5256449865157594	0.6969210118424660	T	T	T
0.3998365374182316	0.4718218819390043	0.7231607756030008	T	T	T
0.7647278693675349	0.1562788592589510	0.6960871536781869	T	T	T
0.2223045333881530	0.9684752783597677	0.2833457400704523	T	T	T
0.2677747556937812	0.7403227049764046	0.3112118789790135	T	T	T
0.5199573104133381	0.0269156341681507	0.3070805877671505	T	T	T
0.6259838856141630	0.1202305593756665	0.3123632394008135	T	T	T
0.7635164279682776	0.7814122941284202	0.3115114064912722	T	T	T
0.7229983170672494	0.5522185279357957	0.2818409705198524	T	T	T
0.0248571922217204	0.4975888183477633	0.3100410866704203	T	T	T
0.9729074706832751	0.2758767726095913	0.2850313313059523	T	T	T
0.5972705443061640	0.2491267157251768	0.6725812443063370	T	T	T
0.6045248007417847	0.6408299319318058	0.6309545394650966	T	T	T
0.6487817750305567	0.6455289705310605	0.5195024736345744	F	F	F
0.6842849885470506	0.8712281182868195	0.3992000288558684	T	T	T

Ti O H Co

1.000000000000000		
14.2453041077000009	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.1680002212999998	0.0000000000000000
0.0000000000000000	0.0000000000000000	29.4789562224999990

Ti O H Fe

21 55 14 3

Selective dynamics

Direct

0.0218388174327543 0.1099047479476565 0.3675649245996758 T T T  
0.1852711252959177 0.6327088861747880 0.3963422399177848 T T T  
0.5218374030958260 0.3961878206928882 0.3656549285998208 T T T  
0.7668602717884998 0.3476255302484663 0.3659525052234894 T T T  
0.9362098341434111 0.6356348837014331 0.3972730248843445 T T T  
0.4408492482741961 0.8640965937434389 0.3988263344116715 T T T  
0.2729119114915269 0.1553964406215383 0.3640329461888694 T T T  
0.7342005810289152 0.1367530326270341 0.4848529224897646 F F F  
0.3956158154875027 0.8683481241609385 0.5172283169192724 F F F  
0.8953822014665107 0.6325289816178099 0.5172296942882255 F F F  
0.2344372928950307 0.3634625181788707 0.4844606095791164 F F F  
0.4815241771643173 0.3615968561732217 0.4834047030315531 F F F  
0.1487325421792534 0.8563983739423122 0.5193773182996253 F F F  
0.9814354254124780 0.1396032612863678 0.4834948480823442 F F F  
0.4419369459753249 0.1399092378544487 0.6067760471510334 T T T  
0.1088033507924127 0.8947577117231503 0.6381443484672480 T T T  
0.9439134786875201 0.3701128214536554 0.6064355523700846 T T T  
0.1878045950813299 0.3680268539437853 0.6050282331504185 T T T  
0.3589581373838168 0.6606442615071917 0.6381388505324693 T T T  
0.8557087071689877 0.8513115793306403 0.6378181813730672 T T T  
0.6869559667220708 0.1385084357389052 0.6033560719758282 T T T  
0.9687695449119978 0.8196278554351916 0.3417494047357328 T T T  
0.7476015739563246 0.1714235403315169 0.4208712497670088 T T T  
0.2509321828585911 0.3127603620053298 0.4210044754035700 T T T  
0.4721895178293846 0.6865462184176511 0.3416676161188079 T T T  
0.8042447659925509 0.6878968905180459 0.3969178495827287 T T T  
0.9001031117717644 0.3174224169346982 0.3646392778655919 T T T  
0.4076410533471140 0.1798201845958263 0.3630624810753413 T T T  
0.3095149719507678 0.8144977656225432 0.3961366559387587 T T T

0.0654083271109860	0.4632545887003540	0.3898035640959014	T	T	T
0.6471603355482582	0.5442559627624998	0.3726209351549669	T	T	T
0.1473766161104782	0.9657313387698280	0.3689729120774381	T	T	T
0.5714760859089639	0.0284906277674222	0.3941512398930128	T	T	T
0.7211302644072020	0.0350471229223921	0.3400007209296359	T	T	T
0.9844346500008182	0.9648734879025220	0.4236391190454106	T	T	T
0.4840273039394817	0.5322246477906762	0.4234170316401190	T	T	T
0.2298721459899308	0.4589121343474813	0.3392096176666917	T	T	T
0.6690919997630900	0.8170932275262288	0.4621108699766978	F	F	F
0.4563443067348629	0.1856957460417874	0.5415381954083784	F	F	F
0.9563715435325619	0.3157762323396867	0.5415514049333012	F	F	F
0.1684768759925106	0.6845410757490313	0.4614047933963619	F	F	F
0.5163401794135183	0.6840621747006708	0.5172222351935218	F	F	F
0.6122121268392959	0.3153938228045661	0.4863254931615089	F	F	F
0.1121104352761861	0.1862923125396918	0.4862169103188876	F	F	F
0.0164653504910319	0.8169379209085434	0.5170864510602016	F	F	F
0.7737086930159478	0.4642121896258828	0.5098542901532497	F	F	F
0.3547568199701061	0.5398845750144545	0.4913055491984935	F	F	F
0.8548352112812623	0.9612879754852131	0.4913474116743402	F	F	F
0.2736558171006749	0.0367285287095171	0.5095842622449496	F	F	F
0.4364578605973435	0.0348585244096000	0.4598389770138454	F	F	F
0.6931547229194095	0.9653791778681509	0.5438751113830449	F	F	F
0.1930960752500894	0.5368671613790212	0.5435284188581946	F	F	F
0.9363025789852344	0.4660265976351923	0.4598071447971463	F	F	F
0.3755547729601648	0.8171887550190101	0.5813013110318532	T	T	T
0.1572274401767323	0.1893717784361448	0.6615200779949597	T	T	T
0.6561310417327267	0.3537960939554986	0.6567637243643192	T	T	T
0.8744380016500317	0.6869602554610603	0.5816199284684221	T	T	T
0.2233532273954881	0.6856296063697009	0.6402785205395016	T	T	T

0.3197173769178839	0.3157052604386085	0.6077113680556844	T	T	T
0.8171217707607974	0.1870118498952082	0.6056923537699763	T	T	T
0.7173769213853334	0.8288563704446072	0.6410196801346385	T	T	T
0.4847149251601549	0.4725451993333329	0.6313072678621303	T	T	T
0.0609076732953213	0.5379470333535993	0.6099479343545841	T	T	T
0.5612470135690140	0.9522491917281988	0.6121893449896554	T	T	T
0.9777540242994566	0.0390406092439488	0.6353651266409291	T	T	T
0.1432787345942537	0.0349714276373473	0.5797246124441175	T	T	T
0.4015850941967898	0.9615629340570788	0.6638154938489060	T	T	T
0.9025663095254102	0.5503903030821713	0.6643308511499626	T	T	T
0.6437111868896950	0.4732060265517534	0.5741827122818746	T	T	T
0.0700265462533625	0.6813874607669879	0.6987688419292061	T	T	T
0.3546732632242786	0.4264008095863374	0.7012736134090796	T	T	T
0.8346841627002960	0.0960753423159396	0.6991287592448284	T	T	T
0.2770159484046392	0.9236609421385960	0.3010495866686777	T	T	T
0.5628321123952044	0.1796307534588831	0.3052503974151254	T	T	T
0.7704375943067937	0.5768382652989982	0.3015632978067724	T	T	T
0.0332918918138812	0.3133834508387294	0.2997270578713572	T	T	T
0.0037601542411865	0.6247090831975847	0.6920238489880657	T	T	T
0.3643684802177812	0.2410921238319522	0.6917403710681704	T	T	T
0.8619993245842009	0.2696910253383696	0.6913777618089827	T	T	T
0.1071751238603009	0.5205736650458819	0.6970053940755159	T	T	T
0.4082997356543990	0.4675822082501374	0.7204386451646231	T	T	T
0.7670878098003389	0.1296240417294850	0.7006479236968546	T	T	T
0.2216636169406981	0.9679419702512768	0.2832232051421140	T	T	T
0.2668827907020709	0.7390315826885562	0.3110367507592989	T	T	T
0.5194456331767457	0.0310947342496999	0.3055862568529998	T	T	T
0.6255857583529634	0.1029397341761282	0.3159704018023566	T	T	T
0.7596865150015902	0.7592669544914009	0.3132839543648624	T	T	T

0.7143826063408214	0.5384128781367834	0.2837880876558822	T	T	T
0.0268985142500541	0.4956689977060710	0.3097596347775591	T	T	T
0.9734665469383239	0.2761022422833438	0.2849666893059720	T	T	T
0.6077034461908571	0.6234286479320147	0.6296704866004152	T	T	T
0.6487817750305567	0.6455289705310605	0.5195024736345744	F	F	F
0.6846243035375214	0.8682975553972546	0.3990676833874017	T	T	T

Ti O Ti O Ti O

1.0000000000000000

14.2453041077000009 0.0000000000000000 0.0000000000000000

0.0000000000000000 5.1680002212999998 0.0000000000000000

0.0000000000000000 0.0000000000000000 29.4789562224999990

Ti O H Fe

21 56 16 3

Selective dynamics

Direct

0.0212509768398770	0.1084129506482283	0.3674090106699419	T	T	T
0.1830964034125851	0.6319524807051046	0.3965298801289899	T	T	T
0.5201665337273591	0.4027422874297855	0.3643336179307512	T	T	T
0.7674446515039280	0.3504375711128989	0.3630083763342225	T	T	T
0.9346191696751630	0.6364302502683462	0.3979408347439988	T	T	T
0.4379631382028067	0.8651111208133164	0.3996682107336942	T	T	T
0.2722578470739169	0.1578319007903199	0.3637936706950959	T	T	T
0.7342005810289152	0.1367530326270341	0.4848529224897646	F	F	F
0.3956158154875027	0.8683481241609385	0.5172283169192724	F	F	F
0.8953822014665107	0.6325289816178099	0.5172296942882255	F	F	F
0.2344372928950307	0.3634625181788707	0.4844606095791164	F	F	F
0.4815241771643173	0.3615968561732217	0.4834047030315531	F	F	F
0.1487325421792534	0.8563983739423122	0.5193773182996253	F	F	F



0.9814354254124780 0.1396032612863678 0.4834948480823442 F F F  
0.4459210189832415 0.1359662140130540 0.6058521092117177 T T T  
0.1046037203785453 0.8936830443295819 0.6350756274086038 T T T  
0.9409481223431504 0.3690831089650718 0.6066536800672303 T T T  
0.1883592310341468 0.3688720258363937 0.6064179988632510 T T T  
0.3587005332824910 0.6527591911894910 0.6363446197365396 T T T  
0.8529273327733994 0.8429111589703387 0.6379415955843764 T T T  
0.6870000316666978 0.1399158574537033 0.6022313622608975 T T T  
0.9697848213157921 0.8182839784670519 0.3417668991289544 T T T  
0.7446824726375341 0.1718735788691008 0.4191619861294658 T T T  
0.2507242601319913 0.3133201272390417 0.4208786429297967 T T T  
0.4706570562939508 0.6913932254000926 0.3410883240691695 T T T  
0.8049843043897879 0.7017492393553874 0.3958897112384792 T T T  
0.9009853729438968 0.3179389820451482 0.3656937361378504 T T T  
0.4079791487203936 0.1804255465096679 0.3635365457523143 T T T  
0.3098137502313233 0.8133938882718509 0.3964068379444614 T T T  
0.0660572703224412 0.4638367400496545 0.3898127216236106 T T T  
0.6473394165483382 0.5513123887105832 0.3709465063373239 T T T  
0.1481178300183597 0.9663188437705180 0.3689289802773588 T T T  
0.5740214219909489 0.0241376271818997 0.3924491561930076 T T T  
0.7283653386806702 0.0755962853524370 0.3298867369716943 T T T  
0.9853159405172855 0.9649958370815789 0.4237497061900758 T T T  
0.4847661160467510 0.5322819549355944 0.4228271182139290 T T T  
0.2305596052138959 0.4602310156144461 0.3389303197976072 T T T  
0.6690919997630900 0.8170932275262288 0.4621108699766978 F F F  
0.4563443067348629 0.1856957460417874 0.5415381954083784 F F F  
0.9563715435325619 0.3157762323396867 0.5415514049333012 F F F  
0.1684768759925106 0.6845410757490313 0.4614047933963619 F F F  
0.5163401794135183 0.6840621747006708 0.5172222351935218 F F F

0.6122121268392959 0.3153938228045661 0.4863254931615089 F F F  
0.1121104352761861 0.1862923125396918 0.4862169103188876 F F F  
0.0164653504910319 0.8169379209085434 0.5170864510602016 F F F  
0.7737086930159478 0.4642121896258828 0.5098542901532497 F F F  
0.3547568199701061 0.5398845750144545 0.4913055491984935 F F F  
0.8548352112812623 0.9612879754852131 0.4913474116743402 F F F  
0.2736558171006749 0.0367285287095171 0.5095842622449496 F F F  
0.4364578605973435 0.0348585244096000 0.4598389770138454 F F F  
0.6931547229194095 0.9653791778681509 0.5438751113830449 F F F  
0.1930960752500894 0.5368671613790212 0.5435284188581946 F F F  
0.9363025789852344 0.4660265976351923 0.4598071447971463 F F F  
0.3740189204001152 0.8179940884215616 0.5810427069672879 T T T  
0.1544937838602803 0.1859405417062420 0.6616327436195262 T T T  
0.6534815411268766 0.3459698846791620 0.6572384152168763 T T T  
0.8755592990012596 0.6876699786880979 0.5811403295640865 T T T  
0.2252989157577980 0.6884621004121965 0.6392426729377769 T T T  
0.3195903978080865 0.3085119385386540 0.6097277818224689 T T T  
0.8170824089157501 0.1878066054585038 0.6070988179716522 T T T  
0.7184398334974440 0.8254031405800800 0.6393187643825742 T T T  
0.4840768136288015 0.4663186866617101 0.6288367424549330 T T T  
0.0605768497602187 0.5413510240490323 0.6126681879120978 T T T  
0.5619413019239405 0.9516992112688447 0.6098957490092053 T T T  
0.9786813257181798 0.0353169566435218 0.6331782155078588 T T T  
0.1441969683799564 0.0383090693857152 0.5791712722195229 T T T  
0.4095621249208401 0.9472802662429973 0.6649196948571130 T T T  
0.8965426611016845 0.5413753263992818 0.6634479567916033 T T T  
0.6432293665089028 0.4789304984545589 0.5775730294802077 T T T  
0.0904037073117369 0.6923504515664388 0.7033244050244185 T T T  
0.3604794296732060 0.4252977023360616 0.7022149444859301 T T T

0.8502569208930295	0.0744906691116257	0.7017215765152456	T	T	T
0.5668875805239427	0.7707573312009512	0.6942168269135971	T	T	T
0.2777446027886346	0.9240064703809204	0.3011358242989635	T	T	T
0.5591659312466472	0.1848178434932370	0.3045407301352471	T	T	T
0.7786964405071627	0.6007615674945097	0.3017322817714513	T	T	T
0.0316132198117793	0.3159293179035734	0.2998869508750254	T	T	T
0.0961936213962000	0.5096691196159396	0.6934347467284327	T	T	T
0.3681730826014391	0.2407691650687370	0.6922592678397600	T	T	T
0.9065974031881557	0.0277170542965017	0.7186146087286868	T	T	T
0.6135786612284838	0.9079774615188746	0.6986599704279486	T	T	T
0.1507408573482755	0.7287463693116062	0.7176796163941517	T	T	T
0.4196334252883646	0.4672873838260572	0.7172147514648739	T	T	T
0.8606961303733769	0.2588168799886438	0.6917574002198498	T	T	T
0.5047554479806156	0.8623501608938671	0.6852322906725983	T	T	T
0.2224915368528370	0.9670790917652071	0.2831514572248460	T	T	T
0.2676150835286636	0.7394544268383444	0.3112641884464781	T	T	T
0.5208734288311628	0.0263252840615063	0.3069943720174149	T	T	T
0.6266131850514282	0.1255601491122940	0.3113623510365718	T	T	T
0.7661537835158151	0.7873951341355200	0.3109469240182960	T	T	T
0.7282570092366329	0.5559503013304620	0.2808533332900407	T	T	T
0.0237526797666892	0.4977642297297104	0.3101027303610667	T	T	T
0.9720306104175787	0.2755698102721899	0.2851408220044965	T	T	T
0.6064676780544558	0.6220032007297368	0.6333830360683007	T	T	T
0.6487817750305567	0.6455289705310605	0.5195024736345744	F	F	F
0.6835247434233824	0.8661903632638358	0.3991260522010146	T	T	T